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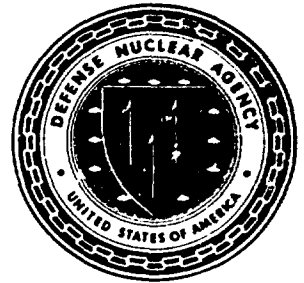**Alexandria, VA 22310-3398**

DNA Chemistry Panel Review—CO$_2$

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December 1990

Technical Report

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13. ABSTRACT *(Maximum 200 words)*
This report is a review of the key parameters involved in the calculation of infrared radiation from CO_2 in a nuclear environment. These parameters include chemical rate coefficients for the formation/destruction of CO_2, rates for collisional excitation/deexcitation of certain vibrational states, and optical parameters including frequencies, Einstein A coefficients and ρB factors for bands of CO_2 originating from vibrational states up to about 5000 cm^{-1}. The rate coefficients are presented in tabular and graphical form and the optical parameters in tabular form. Uncertainty estimates are provided.

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CO_2 vibrational excitation/quenching
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PREFACE

The author is grateful to a number of colleagues at MRC including Mrs. Susan Downer, Drs. Jack Kennealy and Robert Larkin for their helpful suggestions and also, especially, to Dr. Forrest Gilmore (RDA) for his careful review of the preliminary draft of this report and his recommendations for its improvement. Thanks also go to Dr. William Blumberg (GL), Chairman of the DNA Chemistry Panel, and to Dr. Kenneth Schwartz (DNA) for providing the motivation for this work.

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CONVERSION TABLE

Conversion factors for U.S. Customary to metric (SI) units of measurement

MULTIPLY $\longrightarrow$ BY $\longrightarrow$ TO GET

TO GET $\longleftarrow$ BY $\longleftarrow$ DIVIDE

angstrom	1.000000 x E -10	meters (m)
atmosphere (normal)	1.01325 x E +2	kilo pascal (kPa)
bar	1.000000 x E +2	kilo pascal (kPa)
barn	1.000000 x E -28	meter^2 (m^2)
British thermal unit (thermochemical)	1.054350 x E +3	joule (J)
calorie (thermochemical)	4.184000	joule (J)
cal (thermochemical) / cm^2	4.184000 x E -2	mega joule/m^2 (MJ/m^2)
curie	3.700000 x E +1	*giga becquerel (GBq)
degree (angle)	1.745329 x E -2	radian (rad)
degree Farenheit	$t_K = (t_F + 459.67)/1.8$	degree kelvin (K)
electron volt	1.60219 x E -19	joule (J)
erg	1.000000 x E -7	joule (J)
erg/second	1.000000 x E -7	watt (W)
foot	3.048000 x E -1	meter (m)
foot-pound-force	1.355818	joule (J)
gallon (U.S. liquid)	3.785412 x E -3	meter^3 (m^3)
inch	2.540000 x E -2	meter (m)
jerk	1.000000 x E +9	joule (J)
joule/kilogram (J/kg) (radiation dose absorbed)	1.000000	Gray (Gy)
kilotons	4.183	terajoules
kip (1000 lbf)	4.448222 x E +3	newton (N)
kip/inch^2 (ksi)	6.894757 x E +3	kilo pascal (kPa)
ktap	1.000000 x E +2	newton-second/m^2 (N-s/m^2)
micron	1.000000 x E -6	meter (m)
mil	2.540000 x E -5	meter (m)
mile (international)	1.609344 x E +3	meter (m)
ounce	2.834952 x E -2	kilogram (kg)
pound-force (lbs avoirdupois)	4.448222	newton (N)
pound-force inch	1.129848 x E -1	newton-meter (N-m)
pound-force/inch	1.751268 x E +2	newton/meter (N/m)
pound-force/foot^2	4.788026 x E -2	kilo pascal (kPa)
pound-force/inch^2 (psi)	6.894757	kilo pascal (kPa)
pound-mass (lbm avoirdupois)	4.535924 x E -1	kilogram (kg)
pound-mass-foot^2 (moment of inertia)	4.214011 x E -2	kilogram-meter^2 (kg-m^2)
pound-mass/foot^3	1.601846 x E +1	kilogram/meter^3 (kg/m^3)
rad (radiation dose absorbed)	1.000000 x E -2	**Gray (Gy)
roentgen	2.579760 x E -4	coulomb/kilogram (C/kg)
shake	1.000000 x E -8	second (s)
slug	1.459390 x E +1	kilogram (kg)
torr (mm Hg, 0° C)	1.333220 x E -1	kilo pascal (kPa)

*The becquerel (Bq) is the SI unit of radioactivity; 1 Bq = 1 event/s.

**The Gray (Gy) is the SI unit of absorbed radiation.

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SECTION 1

INTRODUCTION

As part of the DNA Chemistry Panel Review, these pages summarize the results of our efforts to provide a reasonably up-to-date compendium of key parameters involved in the calculation of infrared radiation from CO_2 in a nuclear environment. These parameters are: chemical rate-coefficient values (or expressions) for formation/destruction of CO_2, rates for collisional excitation/deexcitation of certain vibrational states and optical parameters including frequencies, Einstein A coefficients and ρB factors for bands of CO_2 originating from vibrational levels up to about 5000 cm^{-1}.

Use has been made of earlier reaction-rate reviews and these have been augmented by our own literature searches of Physics Abstracts through October 1989. Where sufficient data exist to permit it, reaction rates as functions of temperature are presented in graphical form with laboratory data points included. Recommended rate-coefficient expressions are given, where possible, as well as the estimated uncertainty of each. No attempt has been made to provide "guesses" for quantities that may be of interest to the DNA community, such as excitation/deexcitation rate coefficients for certain vibrational states, for which no literature values have been found.

The data are presented in the following order: (1) chemical reaction-rate coefficients, (2) collisional-quenching rate coefficients for CO_2 vibrational states and (3) optical parameters for CO_2 infrared bands.

SECTION 2

CHEMICAL REACTION RATES

The reactions involving the production and destruction of CO_2 considered here are based largely on those in the ARCHON code (Ref. 64) supplemented with a few additional ones involving certain ion-molecule reactions. Table 1 lists the reactions, together with our recommended rate coefficients and suggested uncertainty factors. The rates for the neutral reactions are based on details presented in Figures 1 through 7. A number of the reactions are listed as pairs (a) and (b) with (a) representing the forward (exothermic) reaction and (b) representing the reverse (endothermic) reaction. Most of the rate coefficients are expressed in the standard form [1]

$$k = a(T/300)^b e^{-c/T} \qquad (1)$$

where the constants a, b, c are given in Table 1. Two-body reaction rates have units cm^3 particle $^{-1}sec^{-1}$; three-body rates have units cm^6 particle^{-2} sec^{-1}. The third column in Table 1 lists the exothermicity, ΔE, of each reaction in eV. A negative value for ΔE indicates that the reaction is endothermic by the amount shown.

Uncertainty factors in Table 1 are listed either in the form $(1 \pm x)$, which is self explanatory, or as single factors. In the latter case, an uncertainty factor 2, for example, means that the rate coefficient, k, is estimated to lie within the limits $2k$ and $k/2$. The uncertainty factors are based partially on estimates given in previous literature reviews and partially on "eyeball" estimates of the spread in the experimental data. They pertain to the temperature ranges cited in Table 1. For temperatures outside these ranges, the uncertainties are presumed to be larger.

The last column in Table 1 provides either references for a given reaction rate or else it refers to a specific figure in this report that contains more detailed information about the rate coefficient including data points, temperature plots and references.

Recommended rates, shown in Table 1 and the figures, are weighted more in favor of the later data, especially if the latter show consistency with the principle of detailed balance. A case in point pertains to CO_2 formation and destruction depicted

---

[1] The exception is Reaction 11.

Table 1. CO_2 formation/destruction reactions and rate coefficients.

$$k = a(T/300)^b e^{-c/T}$$

No.	Reaction	ΔE (eV)	a	b	c	Temp. Range (°K)	Uncertainty Factor	Reference/ Comment
1a	$CO + O + N_2 \rightarrow CO_2 + N_2$	5.45	4.9(-33)	-1.44	2191.6	300-6500	2.5	Fig. 1
b	$CO_2 + N_2 \rightarrow CO + O + N_2$	-5.45	9.5(-6)	-2.5	66431.8	300-6500	2	Fig.2
2a	$CO + O + O_2 \rightarrow CO_2 + O_2$	5.45	2.9(-32)	-1.44	2191.6	300-6500	2.5	$6k_{1a}$
b	$CO_2 + O_2 \rightarrow CO + O + O_2$	-5.45	5.7(-5)	-2.5	66431.8	300-6500	3	$6k_{1b}$
3a	$CO + OH \rightarrow H + CO_2$	1.06	2.4(-14)	1.58	-545.5	250-2500	1 ± .5	Fig.3
b	$H + CO_2 \rightarrow CO + OH$	-1.06	7.2(-11)	0.38	12457.0	1000-3000	1 ± .2	Fig.4
4a	$CO + O_2 \rightarrow CO_2 + O$	0.34	1.9(-11)	0	27900	1500-4100	$2(1500/T)^{0.4}$	Fig.5
b	$CO_2 + O \rightarrow CO + O_2$	-0.34	1.3(-10)	0	30400	1500-4100	$2(1500/T)^{0.4}$	Fig.6
5a	$CO + HO_2 \rightarrow CO_2 + OH$	2.71	2.5(-10)	0	11900	700-1000	3	Fig. 7
b	$CO_2 + OH \rightarrow CO + HO_2$	-2.71	9.3(-9)	-0.362	41421	700-1000	3	detailed balance
6	$N(^2D) + CO_2 \rightarrow CO + NO$	3.44	3.5(-12)	0	800	300-1000	1.7	56-61, 65
7	$O^+ + CO_2 \rightarrow (O_2^+ + CO)\cdot$	1.22	9.4(-10)	0	0	300-900	1 ± 0.2	53,54,57,66
8	$N^+ + CO_2 \rightarrow CO_2^+ + N$	0.76	7.5(-10)	0	0	300	1 ± 0.2	54,55,66
	$\rightarrow CO^+ + NO$	4.33	2.5(-10)	0	0	300	1 ± 0.2	54,55,66
9	$N_2^+ + CO_2 \rightarrow CO_2^+ + N_2$	1.81	7.7(-10)	0	0	300	1 ± 0.2	54,66
10	$CO_2^+ + O \rightarrow O_2^+ + CO$	1.37	1.6(-10)	0	0	295	2	62,68
	$\rightarrow O^+ + CO_2$	0.15	9.6(-11)	0	0	295	2	62,66
11	$CO_2^+ + O_2 \rightarrow O_2^+ + CO_2$	1.71	$k = 4.5^{-10} e^{-.0076T} + 7.0^{-12} e^{.0018T}$			94-900	1.4	53,66,67
12	$CO_2^+ + NO \rightarrow NO^+ + CO_2$	4.50	1.2(-10)	0	0	295	1 ± 0.3	62,66
13	$CO_2^+ + e \rightarrow CO + O$	8.32	3.8(-7)	-0.5	0	300	1 ± 0.2	63

* The products of Reaction 7 change from $O_2^+ + CO$ at 300 °K to mainly $CO_2^+ + O$ at 900 °K. In either case, following dissociative recombination, the final products are $CO + 2O$.

3
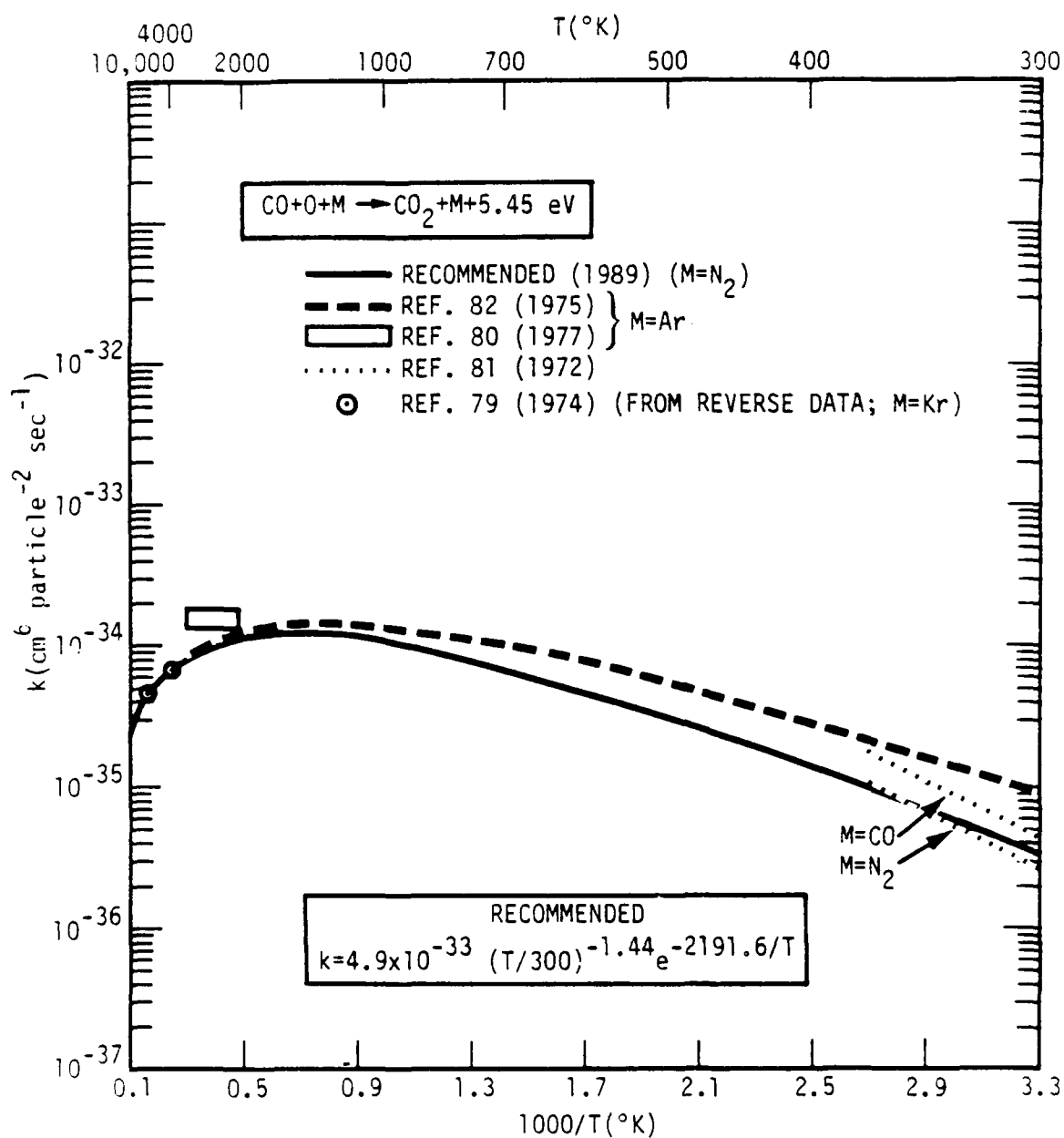
Figure 1. Rate coefficient for the $CO + O + M \rightarrow CO_2 + M$ reaction.

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T(°K)

10,000   7000   5000   4000   3000   2500

$CO_2 + M \longrightarrow CO + O + M \ -5.45 \ eV$

RECOMMENDED (1989)
REF. 48 (1963)
REF. 49 (1964)
⊙ REF. 50 (1965)
X REF. 51 (1966)
□ REF. 52 (1970)
● REF. 79 (1974) M=Kr

$M = N_2$

10^{-12}

10^{-13}

$k(cm^3 \ particle^{-1} \ sec^{-1})$

10^{-14}

10^{-15}

10^{-16}

10^{-17}

RECOMMENDED
$k = 9.5 \times 10^{-6}(T/300)^{-2.5}e^{-66431.8/T}$

10^{-18}

0.1   0.2   0.3   0.4

$1000/T(°K)$
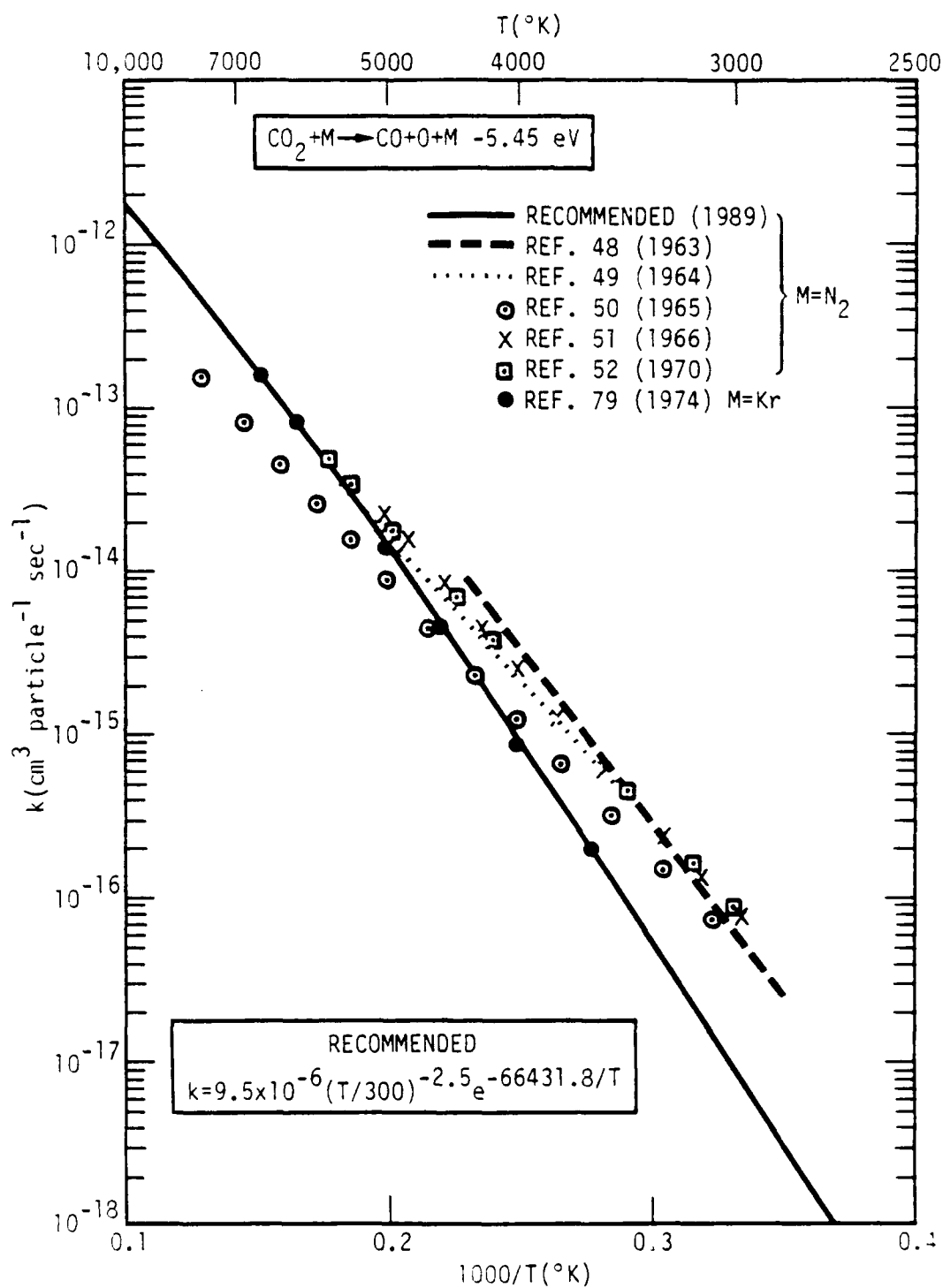
Figure 2. Rate coefficients for the $CO_2 + M \rightarrow CO + O + M$ reaction.
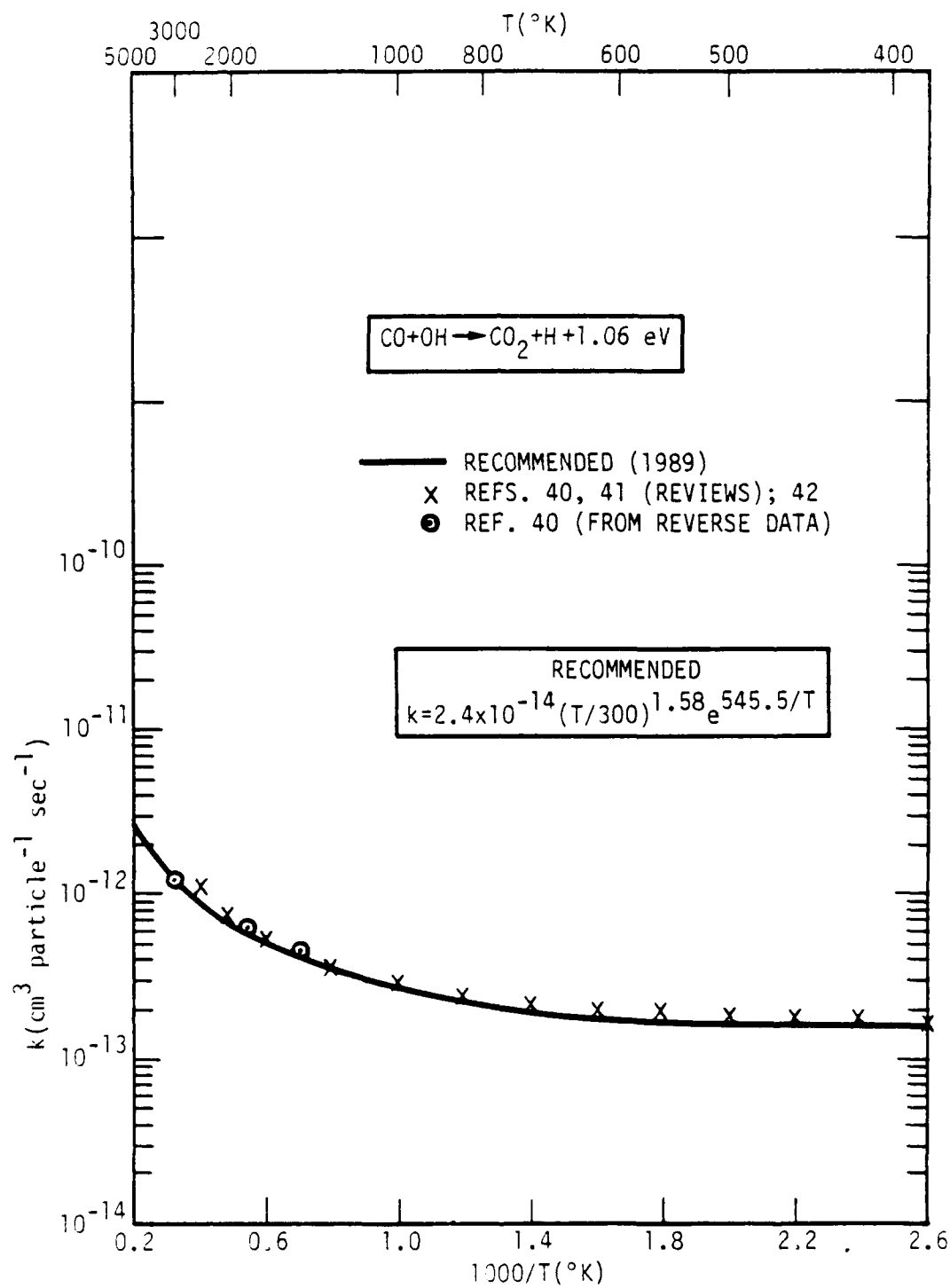
Figure 3. Rate coefficient for the $CO + OH \rightarrow CO_2 + H$ reaction.

6

T($^\circ$K)

3000
5000 2000 1000 800 600 500 400

$CO_2 + H \rightarrow CO + OH - 1.06$ eV

— RECOMMENDED (1989)
⊙ REF. 40 (REVIEW)
X REFS. 40, 41 42 (FROM REVERSE DATA)

RECOMMENDED
$k = 7.2 \times 10^{-11} (T/300)^{0.38} e^{-12457/T}$

10^{-11}
10^{-12}
10^{-13}
10^{-14}
10^{-15}
10^{-16}
10^{-17}

$k(cm^3 particle^{-1} sec^{-1})$

0.2   0.6   1.0   1.4   1.8   2.2   2.6

1000/T($^\circ$K)
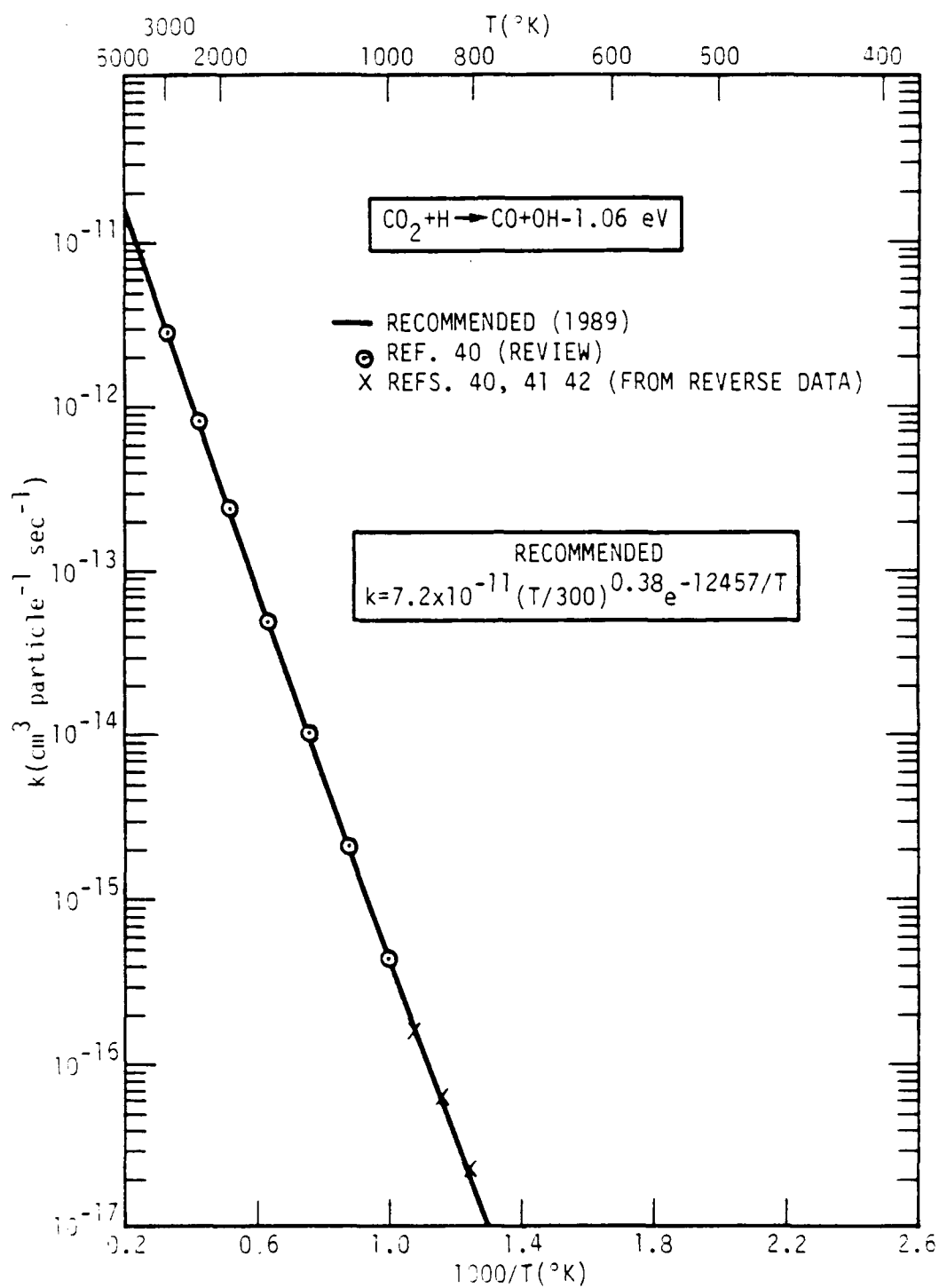
Figure 4. **Rate coefficient for the $CO_2 + H \rightarrow CO + OH$ reaction.**

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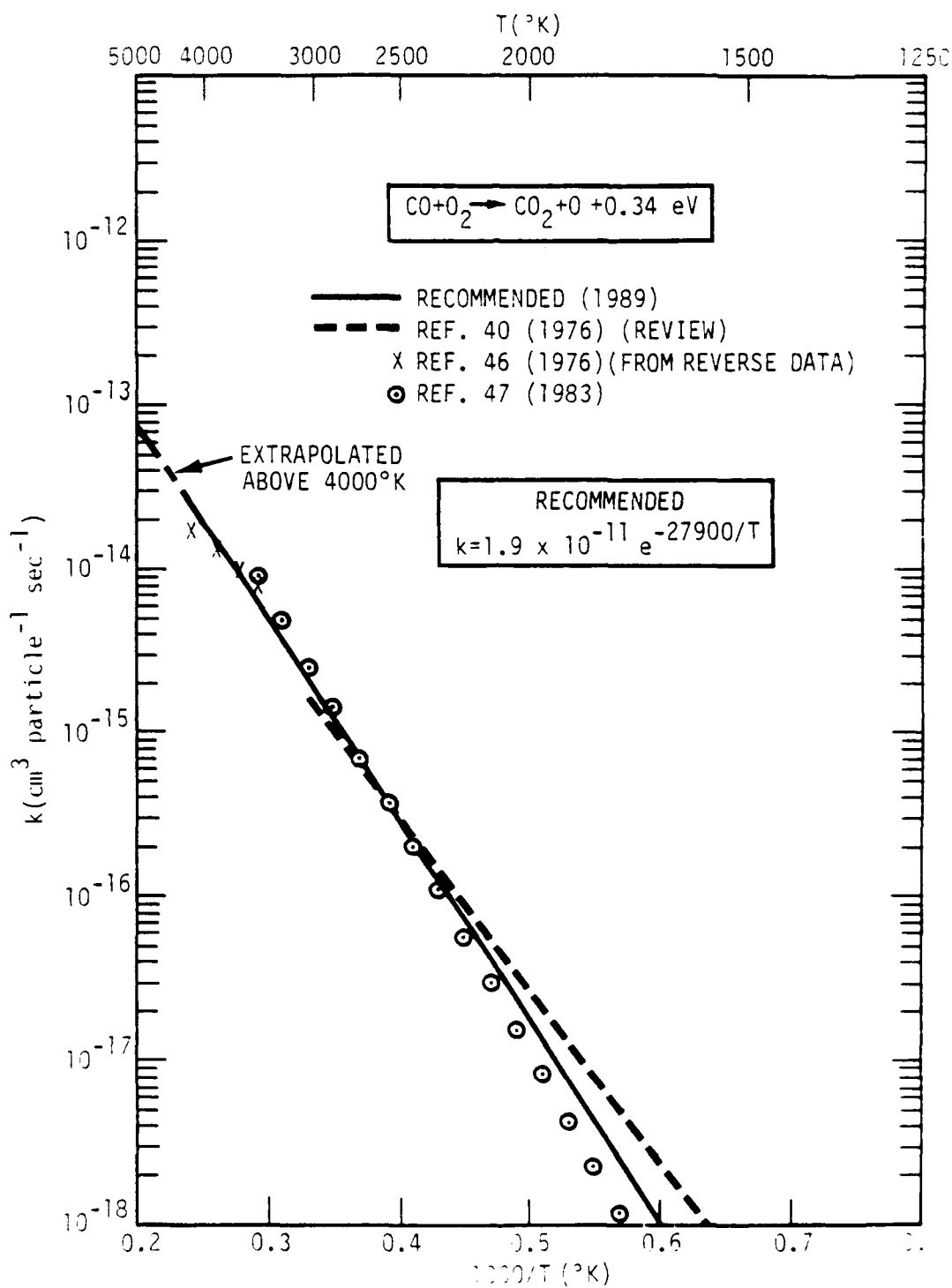
Figure 5. Rate coefficient for the $CO + O_2 \rightarrow CO_2 + O$ reaction.

8
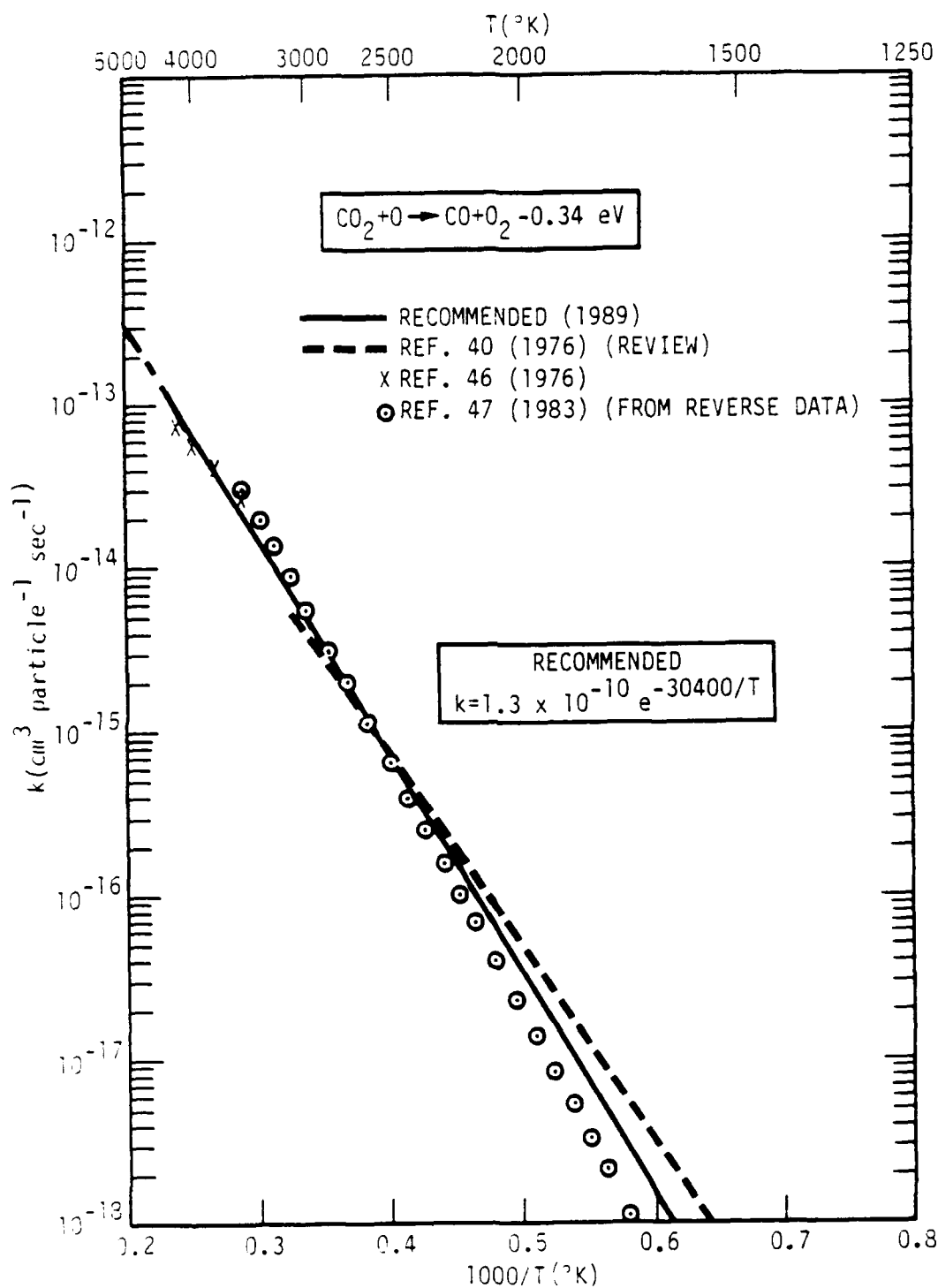
Figure 6. Rate coefficient for the $CO_2 + O \rightarrow CO + O_2$ reaction.

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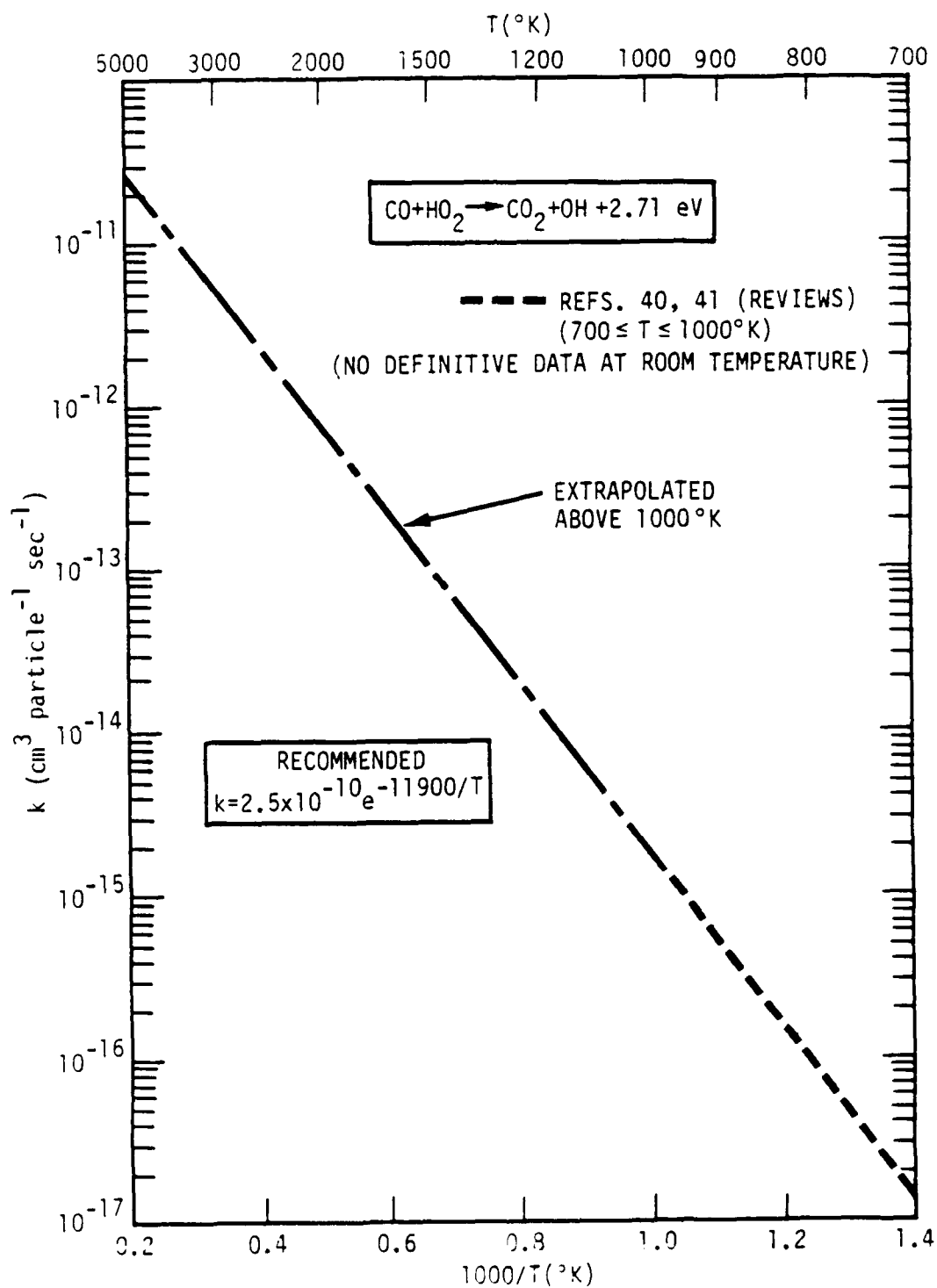
Figure 7. Rate coefficient for the $CO + HO_2 \rightarrow CO_2 + OH$ reaction.

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in Figures 1 and 2, respectively. Much of the older data are unreliable due to the presence of contaminants that the reactions are particularly sensitive to. Some of these older data, relating to CO_2 dissociation at high temperatures, are shown in Figure 2 (References 48 through 52). The newer high-temperature data of Kiefer (Ref. 79) is consistent with the high-temperature rate-coefficient measurements of Dean and Steiner (Ref. 80) for the reverse reaction (Figure 1) and also, through use of classical theory, to measured rates for the reverse reaction at low temperatures. The rate-coefficient expressions in Figures 1 and 2 are consistent with the high-temperature data in References 79 and 80, with the low-temperature data in Reference 81, and with detailed balance through the equilibrium constant as given by the JANAF Tables (Ref. 83). The rate expressions in Figures 1 and 2 apply to $M = N_2$. For $M = O_2$, we adopt a rate that is six times larger (Ref. 39).

SECTION 3

VIBRATIONAL EXCITATION/DEEXCITATION RATES

Recommended excitation/deexcitation rates $(V - T$ and $V - V)$ of CO_2 vibrational states by collisions with major atmospheric species and electrons are presented in Table 2. Our recommendations are based on available data in the literature and on previous reviews. Details, including most of the references, are given in Figures 8 through 17 that are referred to in the "Reference/Comment" column in Table 2. The considerable body of data involving collisions of CO_2 with other CO_2 molecules has been omitted here because of the dominance of CO_2 collisions in the earth's atmosphere with the major species N_2, O_2 and O.

The third column in Table 2 gives the exothermicity, ΔE, of the reactions. Again, negative values for ΔE are given for the endothermic reactions. For Reactions 15 and 22, the exothermicity depends on the ν_2 mode according to the footnotes in Table 2. The symbols (-*) and (-**) in the third column indicate that the values for ΔE are the negative of those in the corresponding footnotes.

The uncertainty factors shown in Table 2 reflect the influence of earlier reviews but are based largely on estimates of the spread in the laboratory data, with heavier weighting generally given to the more recent experiments.

As in Table 1, the forward (exothermic) and reverse (endothermic) reactions in Table 2 are labelled (a) and (b), respectively. Most of the laboratory data pertain to the forward reactions. For the reverse reactions, we have applied the principle of detailed balance to obtain the rate coefficients. For a typical reaction in Table 2 of the form

$$CO_2(v') + A \qquad\qquad CO_2(v'') + B \qquad , \qquad\qquad (2)$$
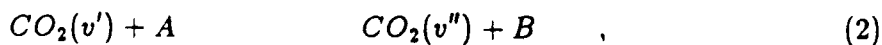
application of this principle leads to a reverse rate coefficient, k_r, in terms of the forward rate coefficient, k_f, given by the expression

$$k_r = \frac{g_{CO_2(v')}}{g_{CO_2(v'')}} e^{-\Delta E / kT} k_f \qquad . \qquad\qquad (3)$$

Table 2. CO_2 vibrational excitation/deexcitation rates.

No.	Reaction	ΔE (eV)	Rate Coefficient (cm^3 sec^{-1})	Temp.Range (°K)	Uncertainty Factor	Reference/Comment
14a	$CO_2(00^01) + N_2 \rightarrow CO_2(00^00) + N_2$	0.291	$k_{14a} = e^{3576.91/T} k_{14b}$	300-8000	1 ± 0.5	detailed balance
14b	$CO_2(00^00) + N_2 \rightarrow CO_2(00^01) + N_2$	-0.291	$1.6 \times 10^{-18} T e^{-3845.23/T}$	300-8000	1 ± 0.5	Fig. 8
15a	$CO_2(00^01) + M \rightarrow CO_2(\nu_2) + M$ $(M = N_2, O_2)$	*	$3.73 \times 10^{-6} e^{-164.47 T^{-1/3}}$ $+1.50 \times 10^{-12} e^{-40.24 T^{-1/3}}$	200-1000	1 ± 0.5	Fig. 9
15b	$CO_2(\nu_2) + M \rightarrow CO_2(00^01) + M$	-*	$k_{15b} = 0.5 e^{-2419.69/T} k_{15a}$	200-1000	1 ± 0.5	detailed balance
16a	$CO_2(00^01) + O \rightarrow CO_2(\nu_2) + O$	*	2×10^{-13}	300	1.2	Fig. 9
16b	$CO_2(\nu_2) + O \rightarrow CO_2(00^01) + O$	-*	$1 \times 10^{-13} e^{-2419.69/T}$	300	1.2	detailed balance
17a	$CO_2(00^01) + N_2(0) \rightarrow CO_2(00^00) + N_2(1)$	0.002	$3.0 \times 10^{-7} e^{-153.51 T^{-1/3}}$ $+5.8 \times 10^{-14} e^{13.73 T^{-1/3}}$	200-3000	1.4	Fig. 10
17b	$CO_2(00^00) + N_2(1) \rightarrow CO_2(00^01) + N_2(0)$	-0.002	$k_{17b} = e^{-27.67/T} k_{17a}$	200-3000	1.4	detailed balance
18a	$CO_2(010) + N_2 \rightarrow CO_2(00^00) + N_2$	0.083	$8.9 \times 10^{-9} e^{-110.04 T^{-1/3}}$ $+1.3 \times 10^{-12} e^{-40.85 T^{-1/3}}$	200-1500	1.3	Fig. 11
18b	$CO_2(00^00) + N_2 \rightarrow CO_2(010) + N_2$	-0.083	$k_{18b} = 2 e^{-960.22/T} k_{18a}$	200-1500	1.3	detailed balance
19a	$CO_2(010) + O_2 \rightarrow CO_2(00^00) + O_2$	0.083	$8.2 \times 10^{-9} e^{-101.87 T^{-1/3}}$ $+1.7 \times 10^{-13} e^{-28.78 T^{-1/3}}$	200-1500	1.3	Fig. 12
19b	$CO_2(00^00) + O_2 \rightarrow CO_2(010) + O_2$	-0.083	$k_{19b} = 2 e^{-960.22/T} k_{19a}$	200-1500	1.3	detailed balance
20a	$CO_2(010) + O \rightarrow CO_2(00^00) + O$	0.083	$k_{20a} = k_{18a} + 3.5 \times 10^{-14} \sqrt{T}$	200-4000	5	Fig. 13
20b	$CO_2(00^00) + O \rightarrow CO_2(010) + O$	-0.083	$k_{20b} = 2 e^{-960.22/T} k_{20a}$	200-4000	5	detailed balance

* For ν_2 = 010, 020, 030, 040; ΔE = 0.209, 0.126, 0.039, -0.040, respectively.

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Table 2. CO_2 vibrational excitation/deexcitation rates (Continued).

No.	Reaction	ΔE (eV)	Rate Coefficient ($cm^3\ sec^{-1}$)	Temp.Range (°K)	Uncertainty Factor	Reference/Comment
21a	$CO_2(020) + N_2 \rightarrow CO_2(010) + N_2$	0.083	$2.8 \times 10^{-8} e^{-110.04T^{-1/3}}$ $+ 4.1 \times 10^{-12} e^{-40.88T^{-1/3}}$	200-1500	2	Fig. 14
21b	$CO_2(010) + N_2 \rightarrow CO_2(020) + N_2$	-0.083	$k_{21b} = e^{-959.11/T} k_{21a}$	200-1500	2	detailed balance
22a	$CO_2(00^00) + O_2(1) \rightarrow CO_2(\nu_2) + O_2(0)$	**	$1.4 \times 10^{-12} e^{-35.85T^{-1/3}}$	200-600	1.5	Fig. 15
22b	$CO_2(\nu_2) + O_2(0) \rightarrow C\dot{O}_2(00^00) + O_2(1)$	-**	$k_{22b} = 0.5 e^{-1279.08/T} k_{22a}$	200-600	1.5	detailed balance
23	$CO_2(100) + M \rightarrow CO_2(020) + M$ $(M = N_2, O_2)$	0.013	2×10^{-11}	300	2.5	Fig. 16
24a	$e + CO_2(010) \rightarrow e + CO_2(00^00)$	0.083	$k_{24a} = 0.5 e^{960.22/T_e} k_{24b}$	200-100,000	2	detailed balance
24b	$e + CO_2(00^00) \rightarrow e + CO_2(010)$	-0.083	$9.6 \times 10^{-8} T_e^{-0.349} e^{-1081/T_e}$ $+ 3.76 \times 10^{-2} T_e^{-1.393} e^{-40869.7/T_e}$	200-100,000	2	Fig. 17
25a	$e + CO_2(00^01) \rightarrow e + CO_2(00^00)$	0.291	$k_{25a} = e^{3370.91/T_e} k_{25b}$	100-100,000	2	detailed balance
25b	$e + CO_2(00^00) \rightarrow e + CO_2(00^01)$	-0.291	$2.0 \times 10^{-7} T_e^{-0.36} e^{-3444.5/T_e}$ $+ 3.86 \times 10^{14} T_e^{-4.683} e^{-171458/T_e}$	100-100,000	2	Fig. 17
26a	$e + CO_2(10^00) \rightarrow e + CO_2(00^00)$	0.172	$k_{26a} = e^{1997.30/T_e} k_{26b}$	200-100,000	2.3	detailed balance
26b	$e + CO_2(00^00) \rightarrow e + CO_2(10^00)$	-0.172	$3.58 \times 10^{-7} T_e^{-0.551} e^{-2168.6/T_e}$ $+ 6.2 \times 10^{-4} T_e^{-1.02} e^{-39304.5/T_e}$	200-100,000	2.3	Fig. 17

** For $\nu_2 = 010, 020$: $\Delta E = 0.110, 0.027$, respectively.
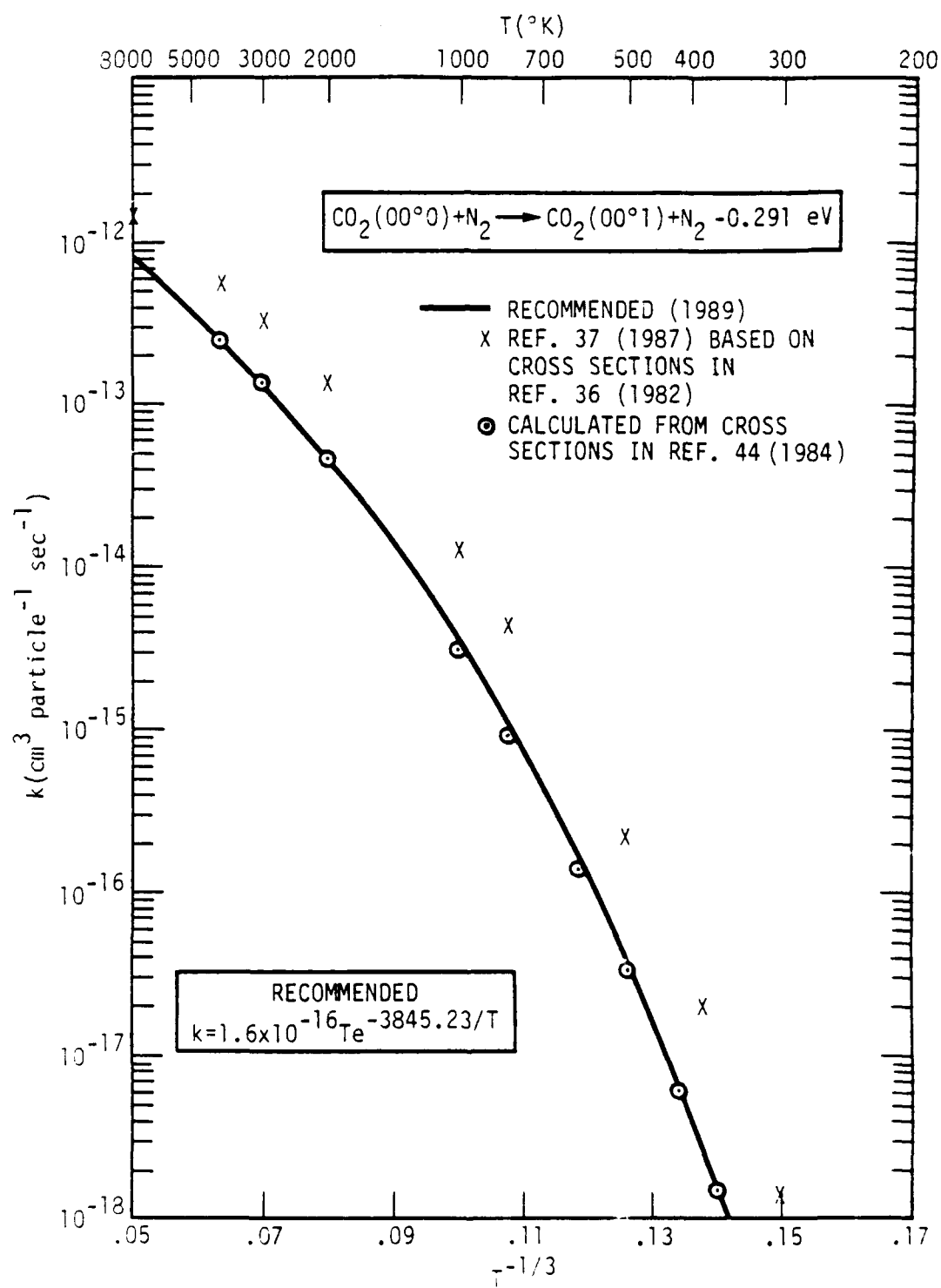
Figure 8. Rate coefficient for the $CO_2(00^00) + N_2 \rightarrow CO_2(00^01) + N_2$ reaction.

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Figure 9. Rate coefficient for the $CO_2(00^01) + M \rightarrow CO_2(\nu_2) + M$ reaction.

16
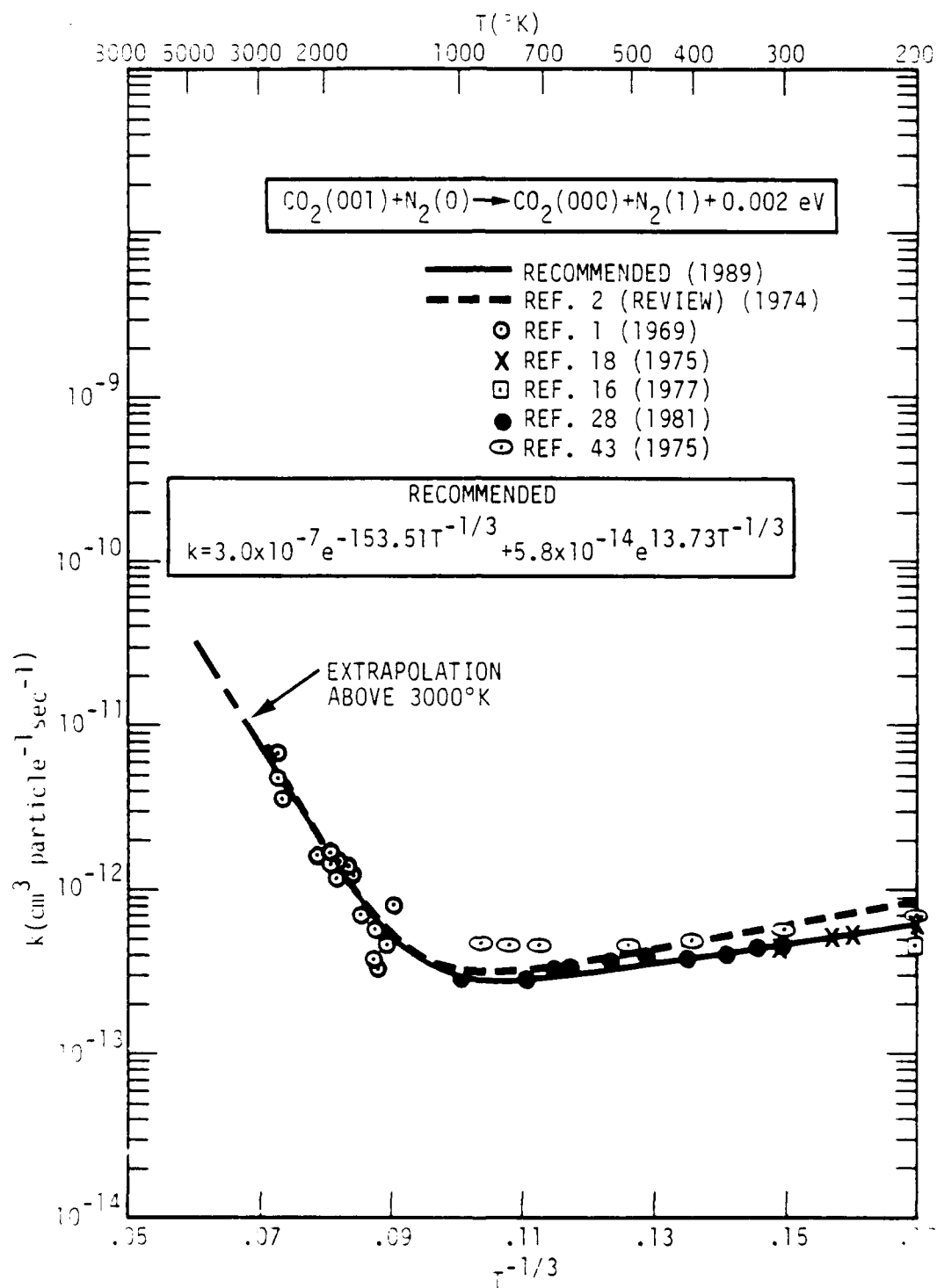
Figure 10. Rate coefficient for the $CO_2(00^01) + N_2(0) \rightarrow CO_2(00^00) + N_2(1)$ reaction.

17
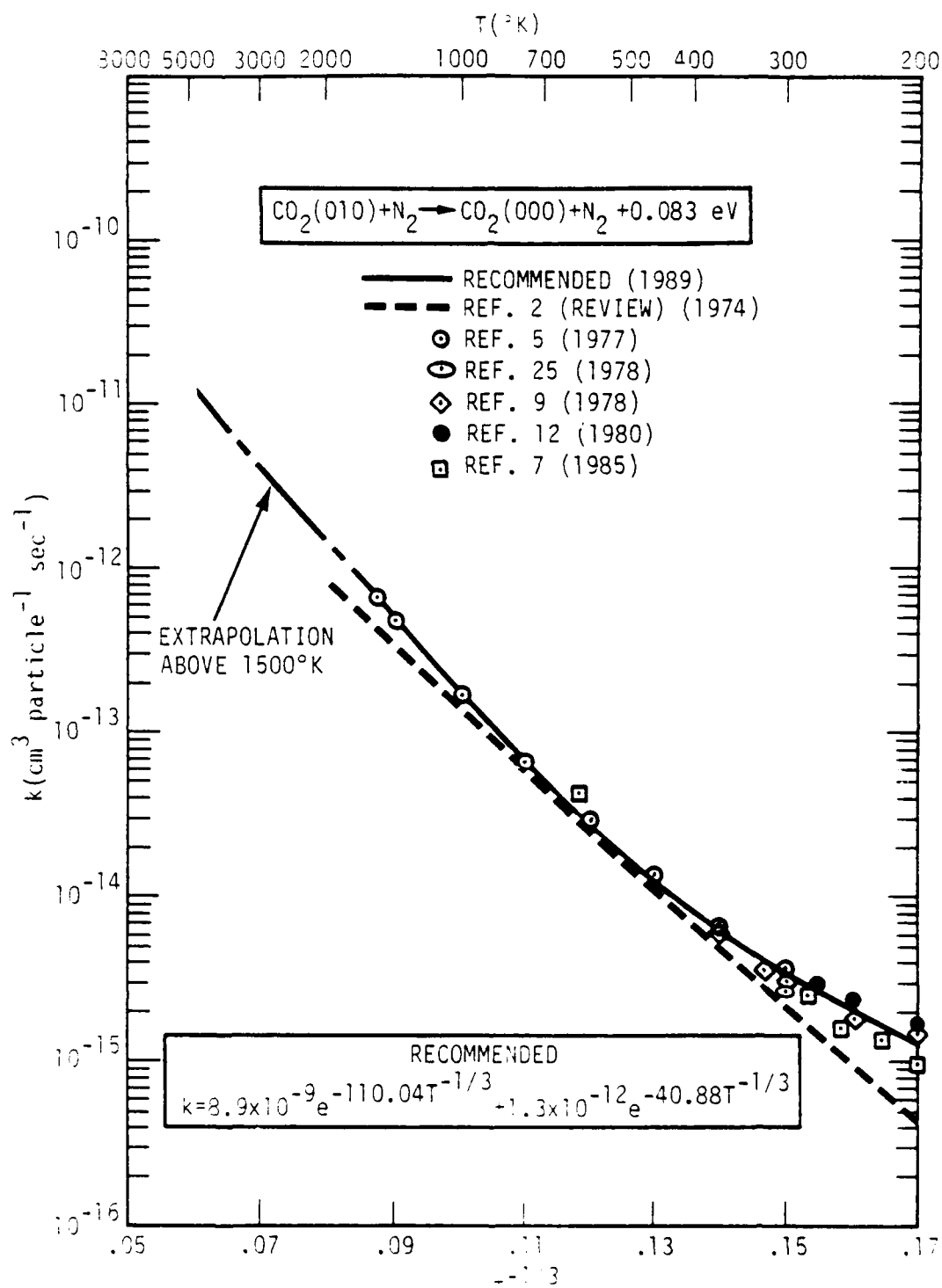
Figure 11. Rate coefficient for the $CO_2(010) + N_2 \rightarrow CO_2(00^00) + N_2$ reaction.

18
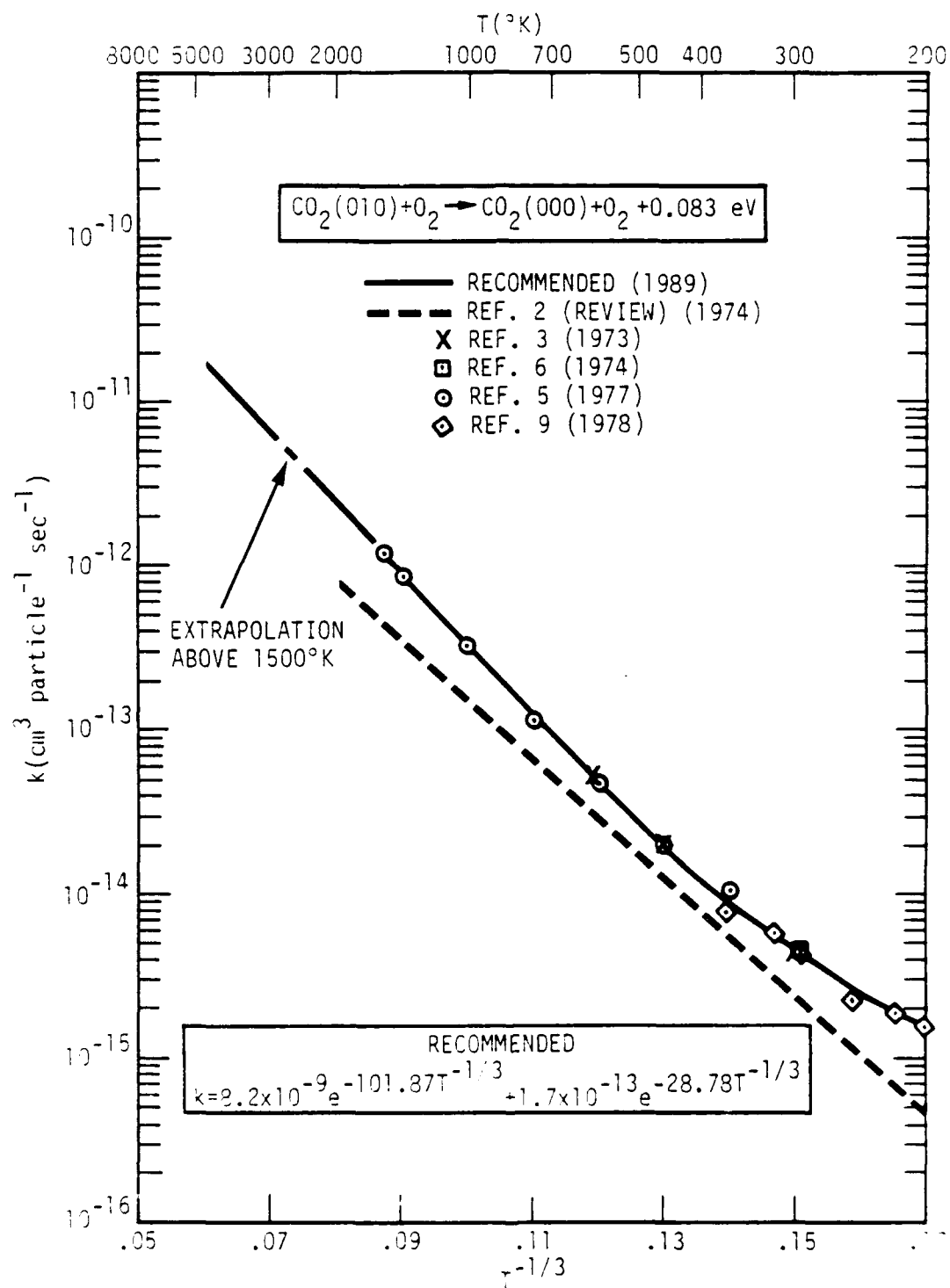
Figure 12. Rate coefficient for the $CO_2(010) + O_2 \rightarrow CO_2(00^00) + O_2$ reaction.

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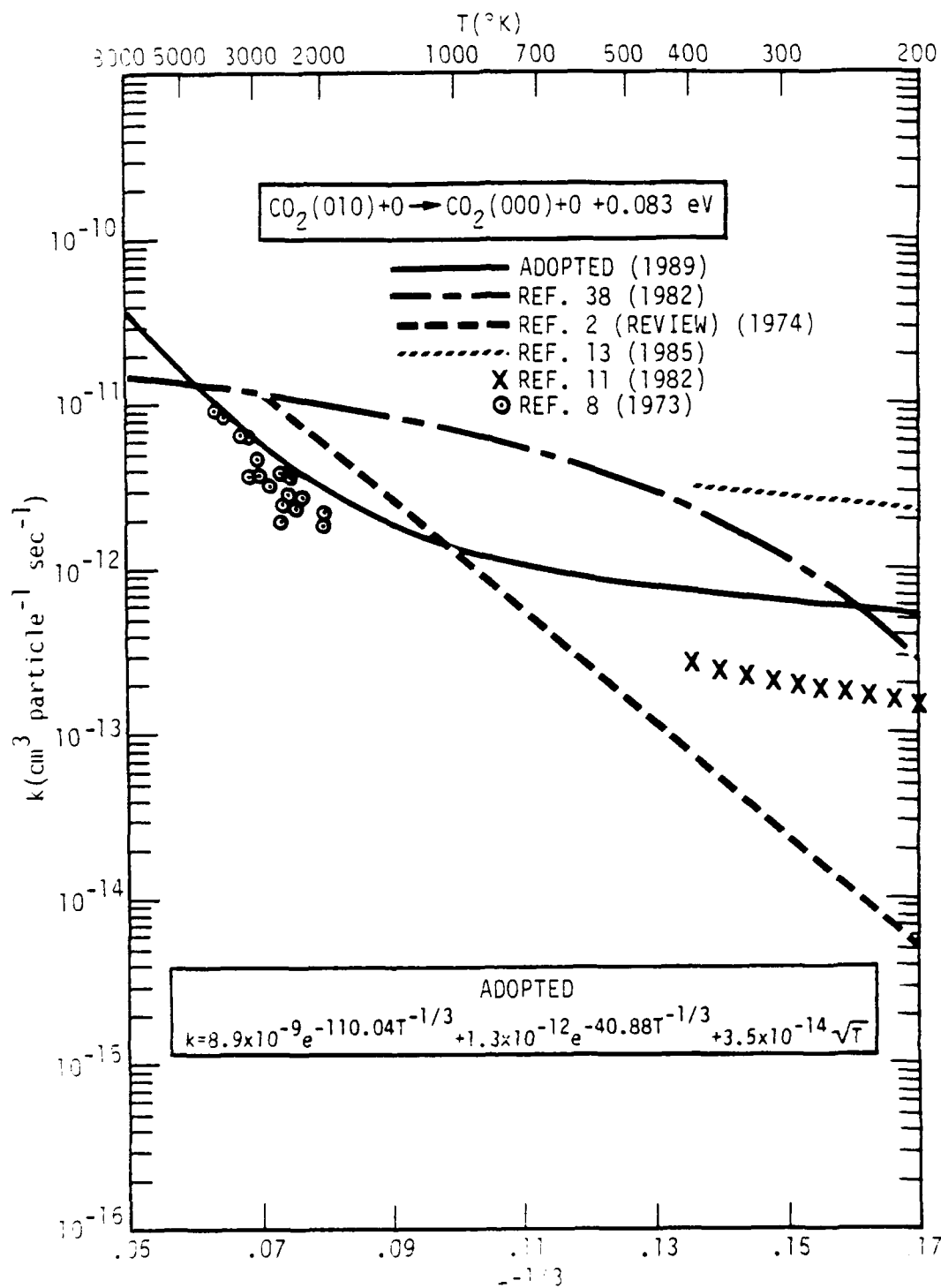
Figure 13. Rate coefficient for the $CO_2(010) + O \rightarrow CO_2(00^00) + O$ reaction.
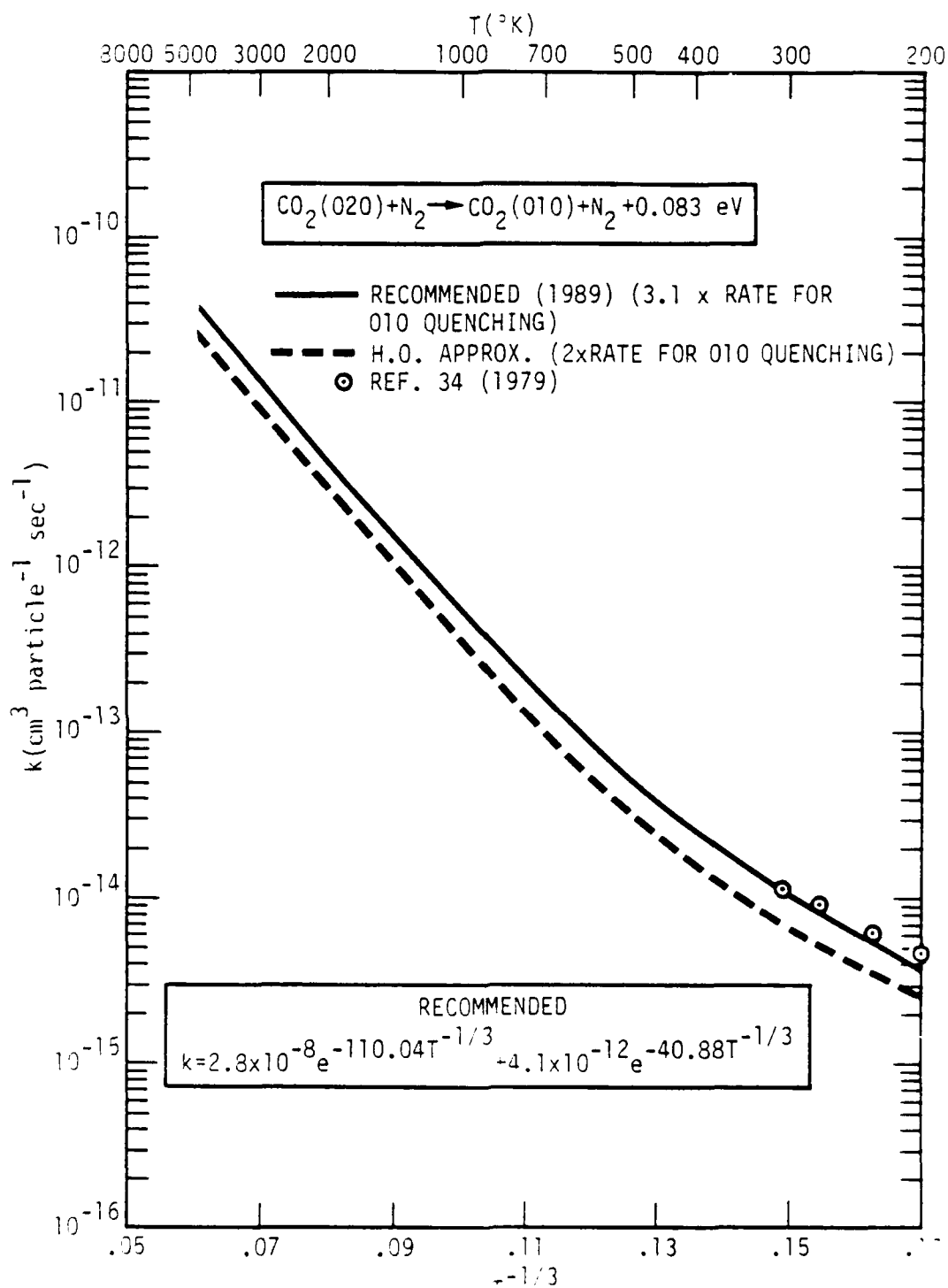
Figure 14. Rate coefficient for the $CO_2(020) + N_2 \rightarrow CO_2(010) + N_2$ reaction.

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T(°K)

3000 5000 3000 2000   1000   700   500 400   300   200

$CO_2(000) + O_2(1) \longrightarrow CO_2(\nu_2)^{**} + O_2(0) + \Delta E$ (SEE TABLE 2)

——— RECOMMENDED (1989)
- - - REF. 2 (REVIEW) (1974)
X   REF. 29 (1969)
⊙   REF. 3 (1973)

10^{-11}

10^{-12}

RECOMMENDED
$k = 1.4 \times 10^{-12} e^{-35.85 T^{-1/3}}$

10^{-13}

$k(cm^3 \ particle^{-1} \ sec^{-1})$

EXTRAPOLATION
ABOVE 600°K

10^{-14}

10^{-15} **VARIOUSLY REPORTED AS 010, 020.

10^{-16}

.05   .07   .09   .11   .13   .15   .17

$T^{-1/3}$
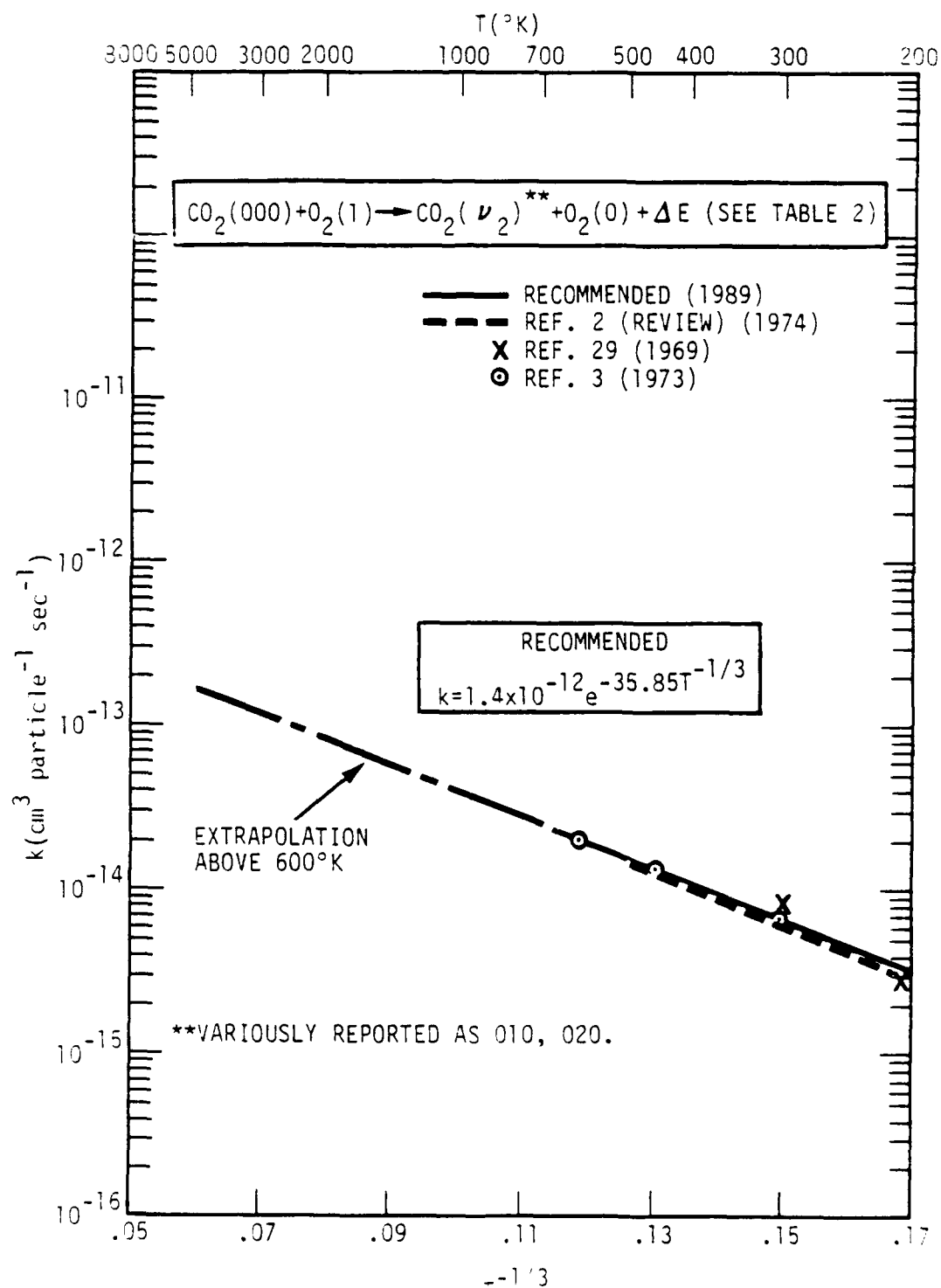
Figure 15. Rate coefficient for the $CO_2(00^0 0) + O_2(1) \rightarrow CO_2(\nu_2) + O_2(0)$ reaction.

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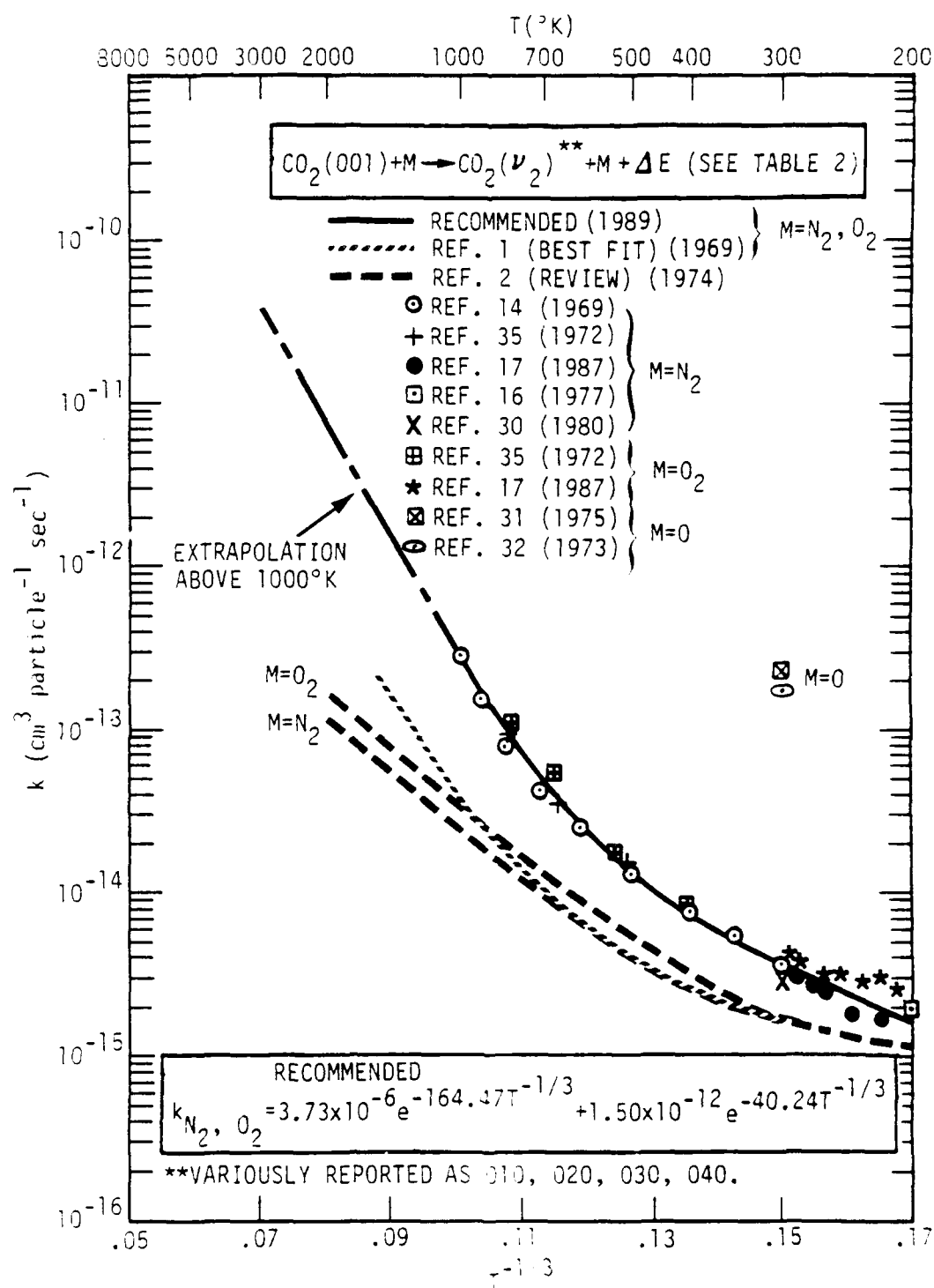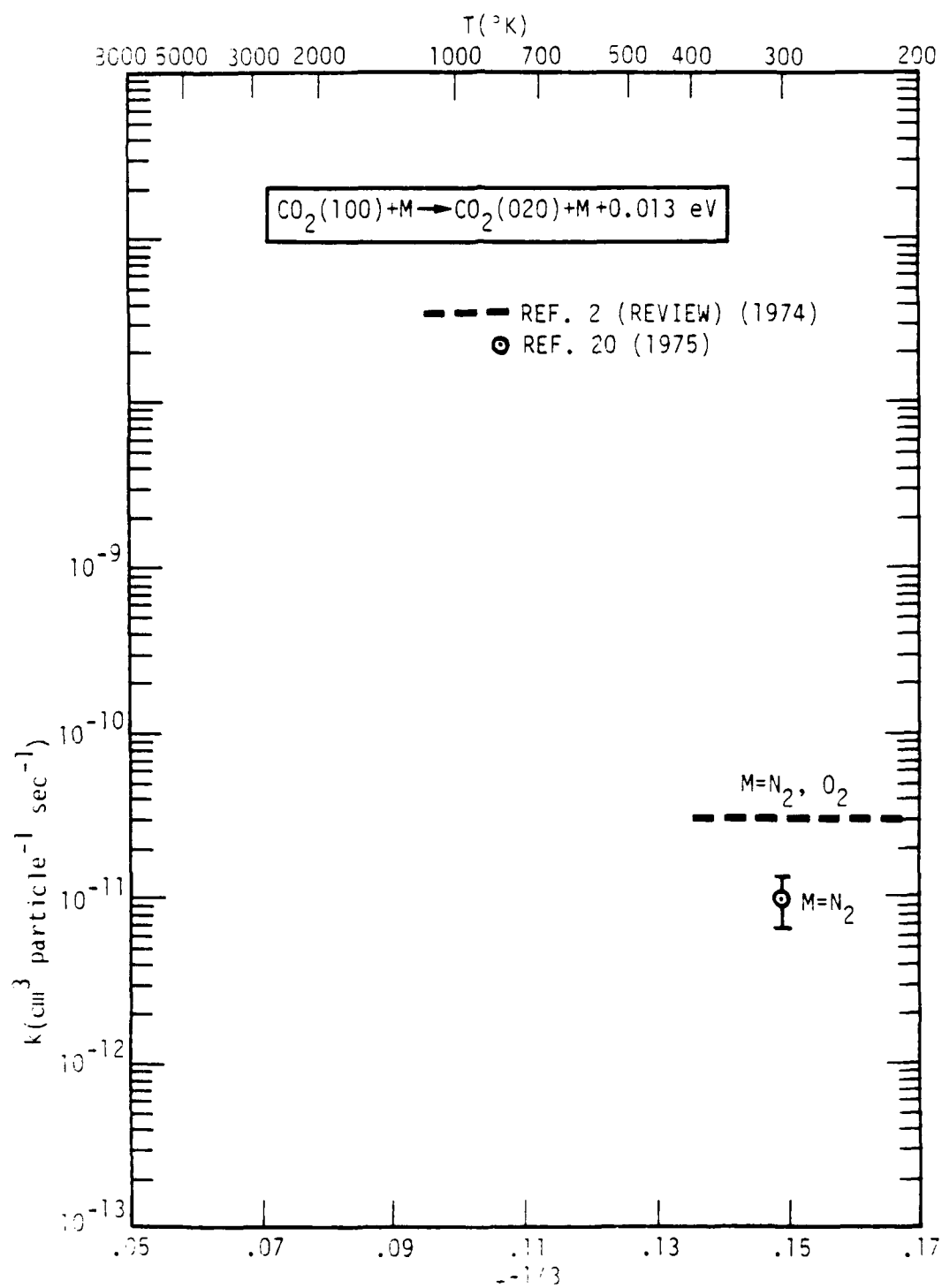**Figure 16.** Rate coefficient for the $CO_2(100) + M \rightarrow CO_2(020) + M$ reaction.
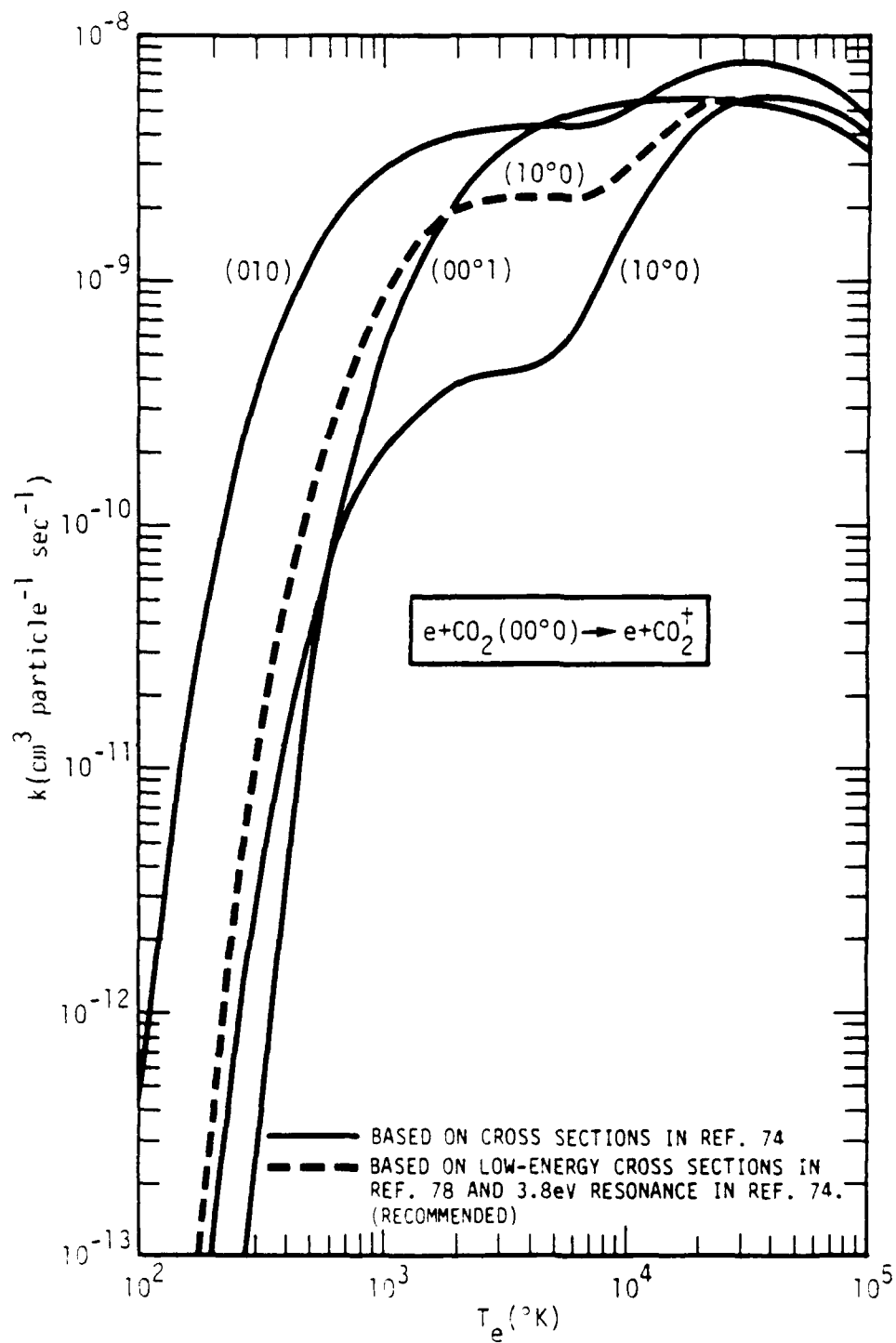
Figure 17. Rate coefficients for the reactions $e + CO_2(00^00) \rightarrow e + CO_2^{\dagger}$.

Here, $g_{CO_2(v')}$ and $g_{CO_2(v'')}$ are the statistical weights of vibrational states v' and v'', respectively, and $\Delta E = E_{v'} + E_A - (E_{v''} + E_B) \geq 0$ is the net endothermicity of the reaction.

For Reaction 14(b), the excitation cross section $\sigma(E)$ has been measured (Refs. 36, 44) as a function of the relative energy, E, of the colliding partners over the energy range from 0.36 to 1.4 eV and we have computed the reaction-rate coefficient as a function of temperature, T, from the relation

$$k = 4.74 \times 10^{11} T^{-3/2} \int_{E_0}^{\infty} E\sigma(E)e^{-11607.54E/T} \, dE \quad (\text{cm}^3\text{sec}^{-1}) \tag{4}$$

where E_0 is the threshold energy, E is in eV units and T is in $^\circ K$. For this calculation we have used the cross sections in Ref. 44 rather than those in Ref. 36 because the latter exhibit considerable scatter. The values of k, for selected values of T, have been fitted by the expression shown in Table 2.

For Reaction 15a in Table 2 (see also Figure 9), our recommended rate-coefficient curve was chosen to fit the larger-valued data points rather than those of some earlier reviews that are not consistent with the later data, especially at the lower temperatures.

For Reactions 24 and 25, involving electron excitation/deexcitation of states 010 and 00^01, we have used the excitation cross sections of Bulos and Phelps (Ref. 74) to calculate the excitation rate coefficients from the formula

$$k = 8.36 \times 10^{13} T_e^{-3/2} \int_{E_0}^{\infty} E\sigma(E)e^{-1.159 \times 10^4 E/T_e} \, dE \quad . \tag{5}$$

Here, E is the electron energy (eV), $\sigma(E)$ is the cross section (cm^2) and T_e is the electron temperature ($^\circ K$). Although these cross sections were determined indirectly from drift-tube measurements in 1976, they are consistent with direct cross-section-measurements by Register et al. (Ref. 75) at 4 and 10 eV and with theoretical calculations for the 00^01 state by Thirumalai and Thuhlar (Ref. 76) at 10 eV. We estimate a factor 2 uncertainty in the cross sections and hence in the rate coefficients.

For Reaction 26, involving electron excitation/deexcitation of state 10^00, the excitation cross sections of Bulos and Phelps below 0.6 eV are about a factor of 4 lower than those calculated by Whitten and Lane (Ref. 77) and measured by Kochem et al. (Ref. 78). Consequently, for the 10^00 state, we have calculated the excitation

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rate coefficient from Equation 5 using (a) the Bulos and Phelps cross sections for both the low-energy region and the higher-energy (3.8 eV "shape resonance") region and (b) the Kochem et al. cross sections for the low-energy region and the Bulos and Phelps cross sections for the higher-energy region. Since the Kochem et al. cross sections (measured only at low energies) are based on direct measurements rather than inferred, as are those of Bulos and Phelps, we recommend results based on the use of the (b) cross sections in Equation 5.

The values for the excitation rate coefficients computed from Equation 5 are shown in Figure 17 for the temperature range 10^2 to 10^5 $°K$. These have been fitted, to within 10 percent, over the indicated temperature ranges by the expressions shown in Table 2 for Reactions 24b, 25b and 26b. In the latter case, the fit has been made to the dashed curve in Figure 17.

SECTION 4

OPTICAL PARAMETERS FOR CO_2 INFRARED BANDS

The optical parameters involved in this review are shown in Tables 3 through 6. These tables include a listing of the vibrational states, their statistical weights and energies up to 5000 cm^{-1} (Table 3), a listing of the bands that arise from transitions between these states (Table 4), and a listing of the wavenumbers, wavelengths, Einstein A coefficients and ρB factors for most of these bands (Tables 5 and 6).

Tables 3 through 6 refer to both individual states and bands and to what are called "composite" states and bands. The latter have been used to advantage in certain models of CO_2 emission, particularly the Delta model (Refs. 71, 72), where a simplification in the number of states and bands to consider is effected by lumping groups of states near the same energy together (including those in Fermi resonance) into a single composite state that has its own energy and statistical weight. Thus, each individual state $(v_1, v_2^\ell v_3)$[1] can be assigned to a composite state $(0mn)$. For m odd, the number of component states is $(m+1)(m+3)/8$. These consist of $(m-1)/2$ subgroups in Fermi resonance + one single state. For m even, the number of component states is $(m+2)(m+4)/8$ consisting of $m/2$ subgroups in Fermi resonance + one single state.

The individual state energies and band frequencies are based on the compilation in Reference 68. The energy, $E_c(\text{cm}^{-1})$, of a composite state appearing in Table 3 is defined in terms of the energies, $E_n(\text{cm}^{-1})$, of the individual states that comprise the composite state by the relation

$$E_c = -\frac{kT}{hc}\ell n \left(\frac{1}{g_c} \sum_n g_n e^{-hcE_n/kT} \right) \qquad , \qquad (6)$$

where g_c, the statistical weight of the composite state, is given by the sum over the individual statistical weights:

$$g_c = \sum_n g_n \qquad . \qquad (7)$$

The values of E_c appearing in Table 3 are for a temperature of 3000 °K.

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[1]In newer terminology, this state would be designated $(v_1 v_2 \ell v_3 r)$ where r is an index indicating the particular Fermi level involved.

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Table 3. Vibrational states and energies of CO_2.

State Notation		Energy (cm^{-1})	g	Composite State	Energy* (cm^{-1})	g_c
old	new					
01^10	01101	667.38	2	010	667.38	2
02^00	10002	1285.41	1			
02^20	02201	1335.13	2	020	1335.65	4
10^00	10001	1388.18	1			
03^10	11102	1932.47	2			
03^30	03301	2003.25	2	030	2035.02	6
11^10	11101	2076.86	2			
00^01	00011	2349.14	1	001	2349.14	1
04^00	20003	2548.37	1			
04^20	12202	2585.02	2			
12^00	20002	2671.14	1	040	2670.75	9
04^40	04401	2671.72	2			
12^20	12201	2760.72	2			
20^00	20001	2797.14	1			
01^11	01111	3004.01	2	011	3004.01	2
05^10	21103	3181.46	2			
05^30	13302	3240.62	2			
13^10	21102	3339.36	2	050	3337.99	12
05^50	05501	3340.72	2			
13^30	13301	3442.22	2			
21^10	21101	3500.67	2			
02^01	10012	3612.84	1			
02^21	02211	3659.27	2	021	3661.23	4
10^01	10011	3714.78	1			
06^00	30004	3792.70	1			
06^20	22203	3821.98	2			
06^40	14402	3898.33	2		-	
14^00	30003	3942.49	1			
14^20	22202	4007.91	2	060	4004.40	16
06^60	06601	4010.07	2			
22^00	30002	4064.27	1			
14^40	14401	4122.27	2			
22^20	22201	4197.36	2			
30^00	30001	4225.10	1			

Table 3. Vibrational states and energies of CO_2 (Continued).

State Notation		Energy	g	Composite	Energy*	g_c
old	new	(cm^{-1})		State	(cm^{-1})	
03^11	11112	4247.71	2			
03^31	03311	4314.91	2	031	4316.93	6
11^11	11111	4390.63	2			
00^02	00021	4673.33	1	002	4673.33	1
07^10	31104	4416.15	2			
07^30	23303	(4474)?	2			
07^50	15502	(4532)?	2			
15^10	31103	4591.12	2			
07^70	07701	(4631)?	2	070	4654.48	20
15^30	23302	(4670)?	2			
15^50	15501	(4710)?	2			
23^10	31102	4753.45	2			
23^30	23301	4890.10	2			
31^10	31101	4938.39	2			
04^01	20013	4853.62	1			
04^21	12212	4887.99	2			
04^41	04411	4970.93	2	041	4973.11	9
12^01	20012	4977.84	1			
12^21	12211	5061.78	2			
20^01	20011	5099.66	1			

*Composite-state energies are weakly temperature dependent. Values shown are for $T = 3000°$ K.

Table 4.   Individual and composite bands of CO_2.

Band	Transition	Composite Band	Transition	Band	Transition	Composite Band	Transition
1	00^01-00^00	1	001-000	26	11^10-10^00	9	030-020
2	00^01-10^00	2	001-020	27	11^10-02^20		
3	00^01-02^00			28	11^10-02^00		
4	02^00-01^10	3	020-010	29	03^10-10^00		
5	02^20-01^10			30	03^10-02^20		
6	10^00-01^10			31	03^10-02^00		
7	01^10-00^00	4	010-000	32	03^30-02^20		
8	10^01-10^00	5	021-020	33	20^00-11^10		
9	10^01-02^00			34	20^00-03^10		
10	02^01-10^00			35	12^00-11^10	10	040-030
11	02^01-02^00			36	12^00-03^10		
12	02^21-02^20			37	04^00-11^10		
13	02^01-00^00	6	021-000	38	04^00-03^10		
14	10^01-00^00			39	12^20-11^10		
15	20^01-00^00	7	041-000	40	12^20-03^30		
16	12^01-00^00			41	12^20-03^10		
17	04^01-00^00			42	04^20-11^10		
18	20^01-10^00	8	041-020	43	04^20-03^30		
19	20^01-02^00			44	04^20-03^10		
20	12^01-10^00			45	04^40-03^30		
21	12^01-02^00			46	01^11-00^01	11	011-001
22	04^01-10^00			47	01^11-11^10	12	011-030
23	04^01-02^00			48	01^11-03^10		
24	12^21-02^20			49	01^11-01^10	13	011-010
25	$04^21\ 02^20$						

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Table 4. Individual and composite bands of CO_2 (Continued).

Band	Transition	Composite Band	Transition
50	21^10–20^00		
51	21^10–12^20		
52	21^10–12^00		
53	13^10–12^20		
54	13^10–12^00		
55	13^10–04^20		
56	13^10–04^00		
57	05^10–04^20	14	050–040
58	05^10–04^00		
59	13^30–12^20		
60	13^30–04^40		
61	13^30–04^20		
62	05^30–04^40		
63	05^30–04^20		
64	05^50–04^40		
65	10^01–01^11	15	021–011
66	02^01–01^11		
67	02^21–01^11		
68	10^01–20^00	16	021–040
69	10^01–12^00		
70	02^01–12^00		
71	02^01–04^00		
72	02^21–12^20		
73	02^21–04^20		

Band	Transition	Composite Band	Transition
74	20^01–20^00		
75	12^01–12^00		
76	04^01–04^00	17	041–040
77	12^21–12^20		
78	04^21–04^20		
79	04^41–04^40		
80	06^60–05^60		
81	06^40–05^60		
82	06^40–05^30	18	060–050
83	06^20–05^30		
84	22^20–21^10		
85	14^40–05^60		
86	06^40–03^30		
87	06^20–03^10		
88	06^00–03^10		
89	14^40–03^30		
90	14^20–03^10		
91	14^20–11^10	19	060–030
92	14^00–03^10		
93	22^00–11^10		
94	22^20–03^30		
95	22^00–03^10		
96	30^00–11^10		
97	06^20–01^10	20	060–010
98	14^20–01^10		

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Table 4.   Individual and composite bands of CO_2 (Continued).

Band	Transition	Composite Band	Transition	Band	Transition	Composite Band	Transition
99	00^02-00^01	21	002-001	107	03^11-01^10	25	031-010
100	00^02-10^01	22	002-021	108	11^11-01^10		
101	00^02-02^01			109	23^10-00^00	26	070-000
102	00^02-01^10	23	002-010				
103	03^11-11^10						
104	03^11-03^10	24	031-030				
105	11^11-11^10						
106	11^11-03^10						

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Table 5. Some optical parameters for individual bands of CO_2 (isotope 626).

BAND	NU (cm-1)	LAMBDA (microns)	A (sec-1)	RHOB(day) (sec-1)	RHOB(night) (sec-1) (optically thin only)
1	2349.14	4.26	4.4178E+02	4.99E-03	1.83E-03
2	960.96	10.41	4.5698E-01	1.93E-03	1.92E-03
3	1063.74	9.40	4.8045E-01	1.21E-03	1.21E-03
4	618.03	16.18	1.2390E+00	1.50E-02	1.49E-02
5	667.75	14.98	3.2313E+00	6.03E-02	6.02E-02
6	720.81	13.87	1.6561E+00	1.18E-02	1.17E-02
7	667.38	14.98	1.5027E+00	5.99E-02	5.98E-02
8	2326.60	4.30	4.1718E+02	4.96E-03	1.93E-03
9	2429.37	4.12	1.6969E-01	1.63E-06	4.70E-07
10	2224.66	4.50	4.3440E-01	6.68E-06	3.34E-06
11	2327.43	4.30	4.1987E+02	4.98E-03	1.93E-03
12	2324.14	4.30	4.2294E+02	5.05E-03	1.98E-03
13	3612.84	2.77	1.1369E+01	4.49E-05	8.67E-08
14	3714.78	2.69	1.8260E+01	6.90E-05	9.38E-08
15	5099.66	1.96	2.3740E-01	5.38E-07	1.10E-12
16	4977.84	2.01	7.3046E-01	1.72E-06	6.20E-12
17	4853.62	2.06	1.5349E-01	3.78E-07	2.42E-12
18	3711.48	2.69	3.0669E+01	1.16E-04	1.43E-07
19	3814.25	2.62	4.1704E-01	1.51E-06	1.17E-09
20	3589.65	2.79	1.5264E+01	6.08E-05	1.31E-07
21	3692.43	2.71	2.2670E+01	8.65E-05	1.16E-07
22	3465.44	2.89	1.4397E-01	6.05E-07	2.29E-09
23	3568.22	2.80	1.7532E+01	7.04E-05	1.67E-07
24	3726.65	2.68	1.9374E+01	7.29E-05	9.38E-08
25	3552.85	2.81	1.0231E+01	4.14E-05	1.05E-07
26	688.67	14.52	2.6132E+00	8.75E-02	8.74E-02
27	741.72	13.48	1.2317E+00	1.57E-02	1.57E-02
28	791.45	12.64	1.2250E-01	2.43E-03	2.42E-03
29	544.29	18.37	3.0947E-02	2.20E-03	2.20E-03
30	597.34	16.74	5.4225E-01	1.46E-02	1.46E-02
31	647.06	15.45	2.1029E+00	8.73E-02	8.72E-02
32	668.12	14.97	4.8912E+00	9.11E-02	9.09E-02
33	720.28	13.88	5.1923E+00	3.70E-02	3.69E-02
34	864.67	11.57	3.2059E-02	1.10E-04	1.09E-04
35	594.29	16.83	6.8899E-01	9.42E-03	9.41E-03
36	738.67	13.54	1.7047E+00	1.11E-02	1.10E-02
37	471.51	21.21	4.3656E-03	1.15E-04	1.15E-04
38	615.90	16.24	2.7670E+00	3.38E-02	3.37E-02
39	683.87	14.62	4.4540E+00	7.65E-02	7.63E-02
40	757.48	13.20	1.3736E+00	1.62E-02	1.61E-02
41	829.26	12.07	1.7654E-03	1.45E-05	1.45E-05
42	508.17	19.68	1.4767E-02	6.39E-04	6.38E-04
43	581.78	17.19	4.9248E-01	1.44E-02	1.44E-02
44	652.55	15.32	3.6875E+00	7.44E-02	7.43E-02
45	668.47	14.96	6.5951E+00	1.23E-01	1.22E-01
46	654.37	15.27	1.5089E+00	6.02E-02	6.01E-02
47	927.16	10.79	3.7035E-01	1.85E-03	1.84E-03
48	1071.54	9.33	4.4585E-01	1.08E-03	1.08E-03
49	2336.63	4.28	4.3196E+02	5.02E-03	1.90E-03
50	703.54	14.21	4.2337E+00	1.31E-01	1.31E-01
51	739.95	13.51	2.7917E+00	3.60E-02	3.59E-02
52	829.53	12.06	1.4686E-01	2.40E-03	2.39E-03
53	578.63	17.28	3.7736E-01	1.12E-02	1.12E-02
54	668.21	14.97	2.6422E+00	9.83E-02	9.82E-02
55	754.34	13.26	1.1277E+00	1.35E-02	1.35E-02

Table 5. Some optical parameters for individual bands of CO_2 (isotope 626)(Continued).

BAND	NU (cm-1)	LAMBDA (microns)	A (sec-1)	RHOB(day) (sec-1)	RHOB(night) (sec-1) (optically thin only)
56	790.99	12.64	3.5165E-01	6.99E-03	6.97E-03
57	596.44	16.77	1.1605E+00	3.14E-02	3.13E-02
58	633.10	15.80	2.7370E+00	1.22E-01	1.22E-01
59	681.49	14.67	6.2469E+00	1.09E-01	1.08E-01
60	770.50	12.98	1.5017E+00	1.66E-02	1.65E-02
61	857.19	11.67	9.8470E-02	7.00E-04	6.38E-04
62	568.91	17.58	4.5210E-01	1.41E-02	1.41E-02
63	655.60	15.25	5.3236E+00	1.06E-01	1.06E-01
64	669.00	14.95	8.3069E+00	1.54E-01	1.54E-01
65	710.77	14.07	1.9375E+00	1.45E-02	1.45E-02
66	608.83	16.42	1.2579E+00	1.59E-02	1.59E-02
67	655.26	15.26	3.1294E+00	6.23E-02	6.22E-02
68	917.65	10.90	5.7305E-01	3.01E-03	2.99E-03
69	1043.64	9.58	6.3937E-01	1.79E-03	1.77E-03
70	941.70	10.62	4.5408E-01	2.11E-03	2.10E-03
71	1064.48	9.39	7.4117E-01	1.87E-03	1.85E-03
72	898.55	11.13	3.3870E-01	1.96E-03	1.95E-03
73	1074.20	9.31	4.3555E-01	1.05E-03	1.04E-03
74	2302.53	4.34	3.9585E+02	4.98E-03	2.06E-03
75	2306.69	4.34	3.9380E+02	4.90E-03	2.01E-03
76	2305.26	4.34	4.0324E+02	5.04E-03	2.07E-03
77	2301.05	4.35	3.9982E+02	5.04E-03	2.10E-03
78	2302.96	4.34	4.0522E+02	5.09E-03	2.11E-03
79	2299.21	4.35	4.0686E+02	5.15E-03	2.16E-03
80	669.35	14.94	1.6950E+01	3.14E-01	3.13E-01
81	557.61	17.93	3.9805E-01	1.32E-02	1.32E-02
82	657.70	15.20	5.7884E+00	1.14E-01	1.14E-01
83	581.36	17.20	1.0015E+00	2.93E-02	2.93E-02
84	696.69	14.35	1.0069E+01	1.62E-01	1.62E-01
85	781.55	12.80	1.5052E+00	1.57E-02	1.56E-02
86	1895.08	5.28	5.0953E-04	2.50E-08	2.02E-08
87	1889.51	5.29	2.2802E-03	1.15E-07	9.31E-08
88	1860.23	5.38	1.3922E-04	3.96E-09	3.29E-09
89	2119.02	4.72	5.8288E-02	1.24E-06	7.58E-07
90	2075.44	4.82	2.2310E-02	5.48E-07	3.61E-07
91	1931.06	5.18	3.1023E-03	1.31E-07	1.03E-07
92	2010.02	4.98	5.2823E-04	8.22E-09	5.91E-09
93	2150.51	4.65	5.5831E-02	1.07E-06	6.21E-07
94	2194.12	4.56	1.2635E-02	2.12E-07	1.13E-07
95	2131.81	4.69	2.2853E-02	2.32E-07	1.39E-07
96	2148.24	4.65	7.2100E-02	6.95E-07	4.05E-07
97	3154.60	3.17	7.9053E-06	3.85E-11	5.91E-13
98	3340.53	2.99	6.6005E-05	2.93E-10	1.95E-12
99	2324.18	4.30	8.3578E+02	9.98E-03	3.91E-03
100	958.54	10.43	8.0982E-01	3.46E-03	3.44E-03
101	1060.49	9.43	8.0224E-01	2.06E-03	2.05E-03
102	4001.95	2.50	2.8183E-04	4.74E-10	1.52E-13
103	2170.85	4.61	2.0366E-01	3.66E-06	2.05E-06
104	2315.24	4.32	4.1240E+02	5.03E-03	2.02E-03
105	2313.77	4.32	4.0841E+02	5.00E-03	2.01E-03
106	2458.16	4.07	4.8311E-02	4.42E-07	1.16E-07
107	3580.33	2.79	1.0733E+01	4.29E-05	9.62E-08
108	3723.25	2.69	1.8899E+01	7.12E-05	8.31E-08
109	4753.45	2.10	2.8195E-06	1.44E-11	1.46E-16

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Table 6. Some optical parameters for composite bands of CO_2 (isotope 626).

COMPOSITE BAND	NU (cm-1)	LAMBDA (microns)	A (sec-1)	RHOB(day) (sec-1) (optically thin only)	RHOB(night) (sec-1) (optically thin only)
1	2349.14	4.26	4.4178E+02	4.99E-03	1.83E-03
2	1011.03	9.89	9.4470E-01	1.55E-03	1.54E-03
3	666.61	15.00	2.3236E+00	8.72E-02	8.71E-02
4	667.38	14.98	1.6027E+00	5.99E-02	5.98E-02
5	2325.56	4.30	4.2089E+02	5.01E-03	1.96E-03
6	3663.10	2.73	1.4679E+01	1.13E-04	1.74E-07
7	4975.01	2.01	3.7164E-01	2.63E-06	9.60E-12
8	3639.76	2.75	2.3419E+01	1.60E-04	2.73E-07
9	668.80	14.95	3.8057E+00	1.06E-01	1.06E-01
10	670.60	14.91	4.8066E+00	1.33E-01	1.32E-01
11	654.87	15.27	1.5089E+00	6.02E-02	6.01E-02
12	1000.82	9.99	8.2909E-01	1.43E-03	1.43E-03
13	2336.63	4.28	4.3196E+02	5.02E-03	1.90E-03
14	672.45	14.87	6.1813E+00	1.50E-01	1.50E-01
15	655.56	15.25	2.3395E+00	9.30E-02	9.28E-02
16	993.20	10.07	1.0039E+00	2.06E-03	2.05E-03
17	2302.32	4.34	4.0186E+02	5.05E-03	2.10E-03
18	669.62	14.93	7.0371E+00	2.17E-01	2.16E-01
19	2021.26	4.95	2.4932E-02	1.74E-06	1.23E-06
20	3244.90	3.08	3.4551E-05	3.22E-10	3.29E-12
21	2324.18	4.30	8.3578E+02	9.98E-03	3.91E-03
22	1006.70	9.93	1.6244E+00	2.73E-03	2.71E-03
23	4005.95	2.50	2.8183E-04	4.74E-10	1.52E-13
24	2314.47	4.32	4.1053E+02	5.02E-03	2.02E-03
25	3650.39	2.74	1.4594E+01	1.13E-04	1.85E-07
26	4753.45	2.10	2.8195E-06	1.44E-11	1.46E-16

The composite-band wavenumbers in Table 6, however, are not determined by simply taking the differences between the composite-state energies shown in Table 3. Rather, they are computed using the method applied to multiplet atomic spectra (Ref. 73). This is because the average frequency, or wavelength, of a composite band depends on the weighting of its constituent bands according to their respective transition probabilities. Specifically, let N be an upper composite state with component states n, and let N' be a lower composite state with component states n'. We then define the average wavelength $\lambda_{NN'}$ and wavenumber $\bar{\nu}_{NN'}$ as follows:

$$\lambda_{nN'} = \frac{\sum_{n'} \lambda_{nn'} A_{nn'}}{\sum_{n'} A_{nn'}} \tag{8}$$

$$\lambda_{NN'} = \frac{\sum_n g_n \lambda_{nN'}}{\sum_n g_n} \tag{9}$$

$$\bar{\nu}_{NN'} = 1/\lambda_{NN'} \quad . \tag{10}$$

The Einstein A coefficients for the individual bands in Table 5 were derived from the band strengths in Reference 68 using the relation (Refs. 69, 70) [2]

$$A_{nm} = 7.540 \times 10^{11} \frac{\bar{\nu}_{nm}^2 Q_V(T_0) S_v^0 e^{c_2 E_m/T_0}}{g_n I_a (1 - e^{-c_2 \bar{\nu}_{nm}/T_0})} \quad . \tag{11}$$

Here, $Q_V(T_0)$ is the vibrational partition function for CO_2 at temperature $T_0 = 296°K$ (taken to be 1.0931), c_2 is the second radiation constant ($hc/k = 1.43879$), E_m is the energy (cm^{-1}) of the lower state, g_n is the statistical weight of the upper state, I_a is the isotopic abundance, and S_v^0 is the band strength, in units of cm^{-1}/(molecule cm^{-2}), tabulated in Reference 68. Tables 5 and 6 pertain to the major isotope (626) with abundance 0.98414.

The Einstein A coefficients in Table 6 for the composite bands are defined in terms of the A values and wavelengths of the component bands by the relation

$$A_{NN'} = \frac{\sum_{n,n'} g_n \lambda_{nn'}^3 A_{nn'}}{\lambda_{NN'}^3 \sum_n g_n} \quad . \tag{12}$$

---

[2]Equation 10 in Reference 68 should not contain the factor g'' and Equation 1 in Reference 69 should not contain the factor g_i.

The factors ρB are the product of the radiation field density (at wavenumber $\bar{\nu}_{nm}$) and the Einstein B coefficient for absorption and represent the rate ($\sec^{-1}$ molecule $^{-1}$) at which the radiation field induces transitions from the lower state m to the upper state n. The values are given for day and night conditions and assume optical thinness. The nighttime values, based on earthshine from a flat black body earth at temperature $T_E(288°K)$ radiating into 2π steradians, can be represented by the equation (Ref. 71)

$$(\rho B)^E = \frac{1}{2}(g_n/g_m)A_{nm}\left(e^{c_2\bar{\nu}_{nm}/T_E} - 1\right)^{-1} \quad . \tag{13}$$

For sunlight conditions, we assume a 6000 °K black-body sun that subtends a solid angle of 6.8×10^{-5} ster at the earth. The appropriate equation (Ref. 71) is

$$(\rho B)^S = 5.4 \times 10^{-6}(g_n/g_m)A_{nm}\left(e^{2.391\times 10^{-4}\bar{\nu}_{nm}} - 1\right)^{-1} \quad . \tag{14}$$

The daytime values for ρB are given by the sum of Equations 13 and 14.

We emphasize that Equations 13 and 14 are valid only for optically-thin conditions for which attenuation of earthshine by the atmosphere above the earth's surface, and of sunlight below the top of the atmosphere, are negligible. These conditions are severely violated for the stronger bands of CO_2, especially for the ν_2 and ν_3 transitions that terminate on the ground state (individual bands 1 and 7 in Table 4). For these and other bands that may be optically thick, transmission effects cannot be neglected and the energy density of the radiation field from the external sources (earth and sun) is altitude dependent. The values for ρB given in Tables 5 and 6 are based on Equations 13 and 14 and, as such, they disregard the issue of optical thickness. For those bands that are optically thick (particularly bands 1 and 7 in Table 5 and 1 and 4 in Table 6), the ρB values should be considered as upper limits.

As to the uncertainty in the parameter values shown in Tables 3, 5 and 6, Reference 68, that forms the basis for most of these values, states that the individual energy levels and band wavenumbers are good to within 0.001 cm^{-1}, and the band intensities (and hence Einstein coefficients) to about 10 percent.

SECTION 5

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